Parallel Eigensolvers for a Discretized Radiative Transfer Problem

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The Radioative Transfer Problem

We want to solve $T\varphi = \theta\varphi$ where

- T is an integral operator defined on $X = L^1(I), I = [0,\tau^*]$

$$(Tx)(\tau) = \int_{\tau^*} g(|\tau - \tau'|)\, x(\tau')\, d\tau'$$

- τ is the optical depth of a stellar atmosphere
- τ^* optical thickness of the atmosphere
- g is the kernel $g(\tau) := \dfrac{\varpi}{2} \underbrace{\int_1^\infty \dfrac{\exp(-\tau\mu)}{\mu} d\mu}_{E_1}, \tau > 0$
- and $\varpi \in]0,1[$ is the albedo[a]

E_1 first exponential-integral function

[a] Reflective power

Projection method (Kantorovich) and matrix formulation

$$T\varphi = \theta\varphi$$

approximate by

$$T_m\varphi_m = \theta_m\varphi_m$$

leads to the solution of a finite dimensional eigenproblem

$$Ax = \lambda x$$

$$0 = \tau_{m,0} < \tau_{m,1} < \cdots < \tau_{m,m-1} < \tau_{m,m} = \tau^*$$

$$e_{m,j} \in X, \quad e_{m,j} = \begin{cases} 1, & \tau \in]\tau_{m,j-1}, \tau_{m,j}[\\ 0, & \tau \notin]\tau_{m,j-1}, \tau_{m,j}[\end{cases}$$

$$X_m = span\left\{ e_{m,j},\ j = 1,\ldots,m \right\}$$

π_m projection op. $\pi_m\ x = \sum_{j=1}^{m} \left\langle x, e^*_{m,j} \right\rangle e_{m,j}$

$$T_m x = \pi_m T x = \sum_{j=1}^{m} \left\langle x, T^* e^*_{m,j} \right\rangle e_{mj}$$

A is the restriction of T_m to X_m : $A = \left(\left\langle e_{m,j}, T^* e^*_{m,i} \right\rangle \right)_{i,j=1}^{m}$

$e^*_{m,j}$ is the adjoint basis of $e_{m,j}$ in X^*

Matrix Coefficients

grid $\left(\tau_{m,j}\right)_{j=0}^{m}$ defined on $\left[0,\tau^*\right]$, for $i, j \in [1, m]$

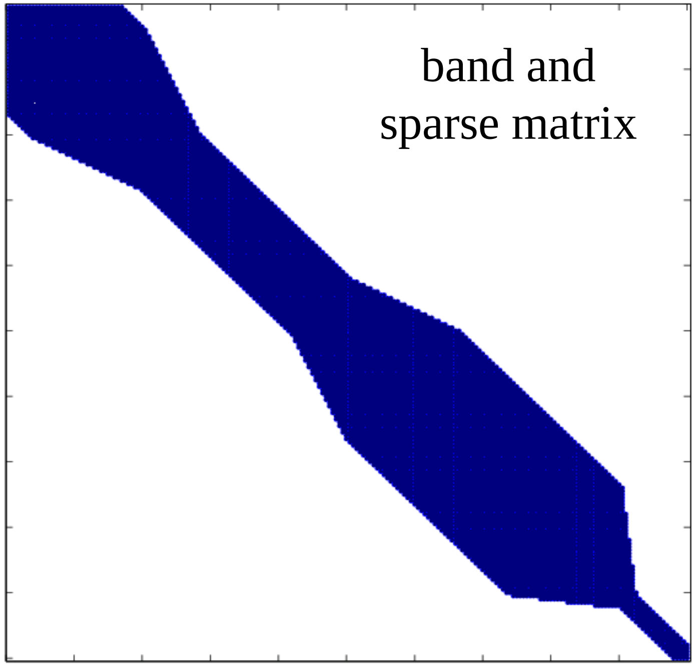
$$A(i,j) = \frac{\varpi}{2h_{m,i}} \int_{\tau_{m,i-1}}^{\tau_{m,i}} \int_0^{\tau^*} E_1\left(\left|\tau - \tau'\right|\right) e_{m,j}(\tau')\, d\tau'\, d\tau$$

$$= \begin{cases} \dfrac{\varpi}{2h_{m,i}}\left[E_3\left(d_{m,i-1,j}\right) - E_3\left(d_{m,i-1,j-1}\right) + E_3\left(d_{m,i,j-1}\right) - E_3\left(d_{m,i,j}\right)\right], & i \neq j \\ \varpi\left(1 + \dfrac{1}{h_{m,j}}\left[E_3\left(h_{m,j} - \dfrac{1}{2}\right)\right]\right), & i = j \end{cases}$$

$$d_{m,i,j} = \left|\tau_{m,i} - \tau_{m,j}\right|, \; i,j \in [0, m]$$

$$h_{m,j} = \tau_{m,j} - \tau_{m,j-1}, \; j \in [1, m]$$

$$E_3(\tau) := \int_1^{\infty} \frac{\exp(-\tau\mu)}{\mu^3}\, d\mu, \; \tau > 0$$



Solution strategies

- We can approximate $T_m\,\varphi_m = \theta_m \varphi_m$ by solving the matrix problem $Ax=\lambda x$ for large values of m
- Our goal is to experiment with robust and portable algorithmic implementations (from the ACTS Collection)
- Direct methods:
  - ScaLAPACK: *pdsyevx* (bisection + inverse iteration)
- Iterative methods:
  - SLEPc: Arnoldi, Krylov-Schur[a], interface to PRIMME[b], etc

[a] Krylov-Schur is equivalent to implicit restarted Arnoldi

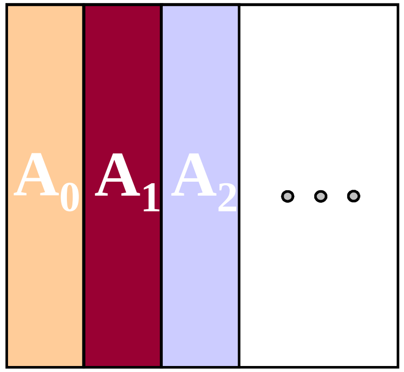
[b] PReconditioned Iterative MultiMethod Eigensolver

Hardware and problem specification

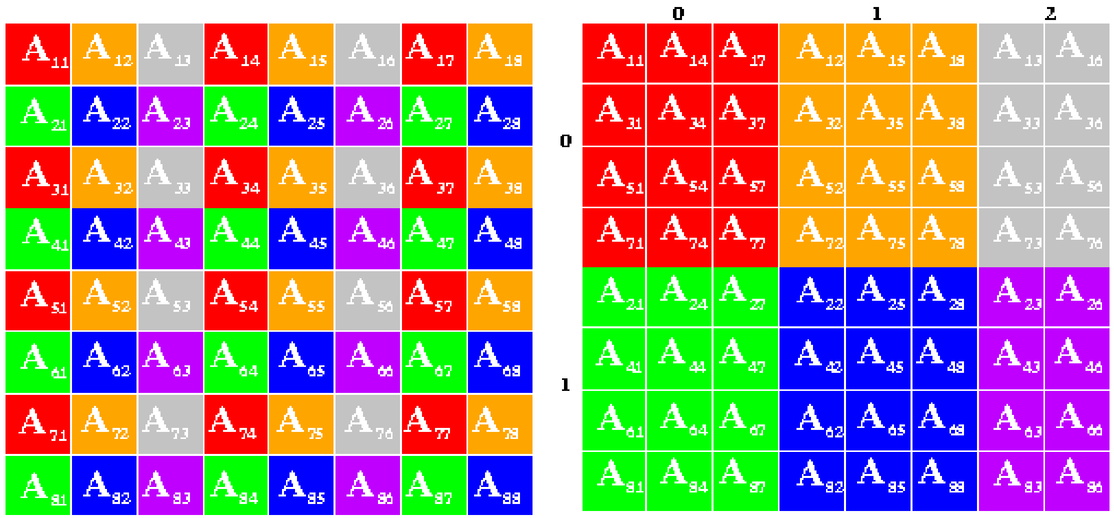
- LBNL/NERSC:
  - Jacquard – AMD Opteron cluster: 356 dual-processor nodes, 2.2 GHz/node, 6 GB/node, interconnected with a high-speed InfiniBand network. ACML library.
  - Bassi – IBM SP5: 122 compute nodes with 8 1.9 GHz Power 5 processors/node, 32 GB memory/node. ESSL library.
- Universidad Politécnica de Valencia:
  - Odin – Pentium Xeon cluster: 55 dual-processor nodes, 2.2 GHZ processors, 1 GB/node, interconnected with a high-speed SCI network with 2-D torus topology.
- problem specification:
  - $\varpi=0.75$, $tol \leq 10^{-12}$ (similar computation times for larger ϖ)

ScaLAPACK data distribution

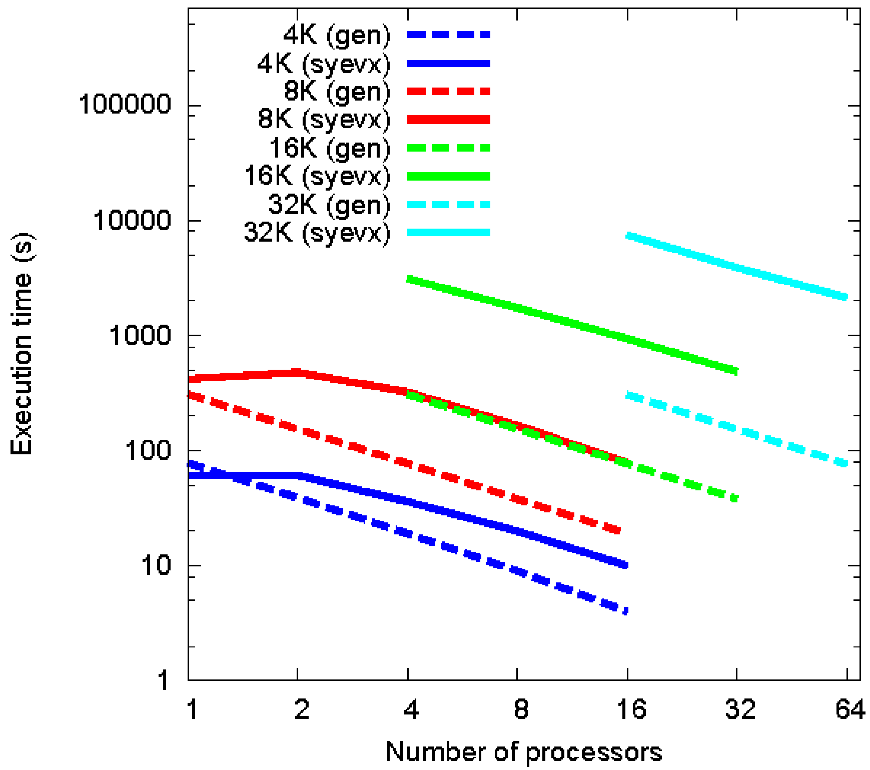
- 1-dimensional block-column distribution (for narrow band matrices)



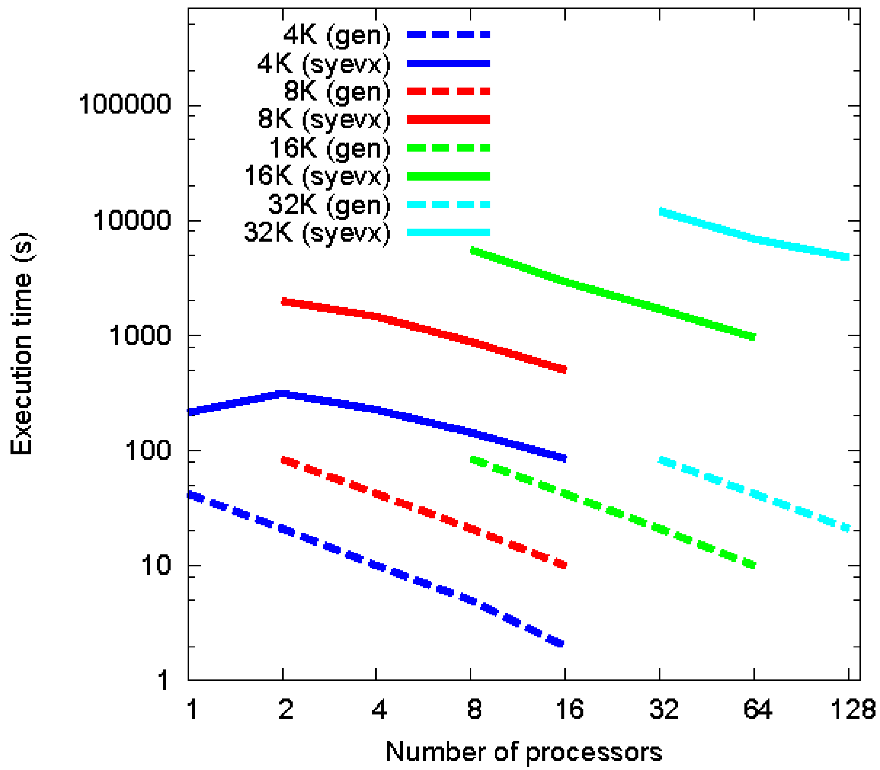
- 2-dimensional block cyclic distribution (for general dense matrices)



ScaLAPACK: *times* on bassi and jacquard



Execution times for the matrix generation and eigensolution phases on bassi; all eigenvalues but no eigenvectors.



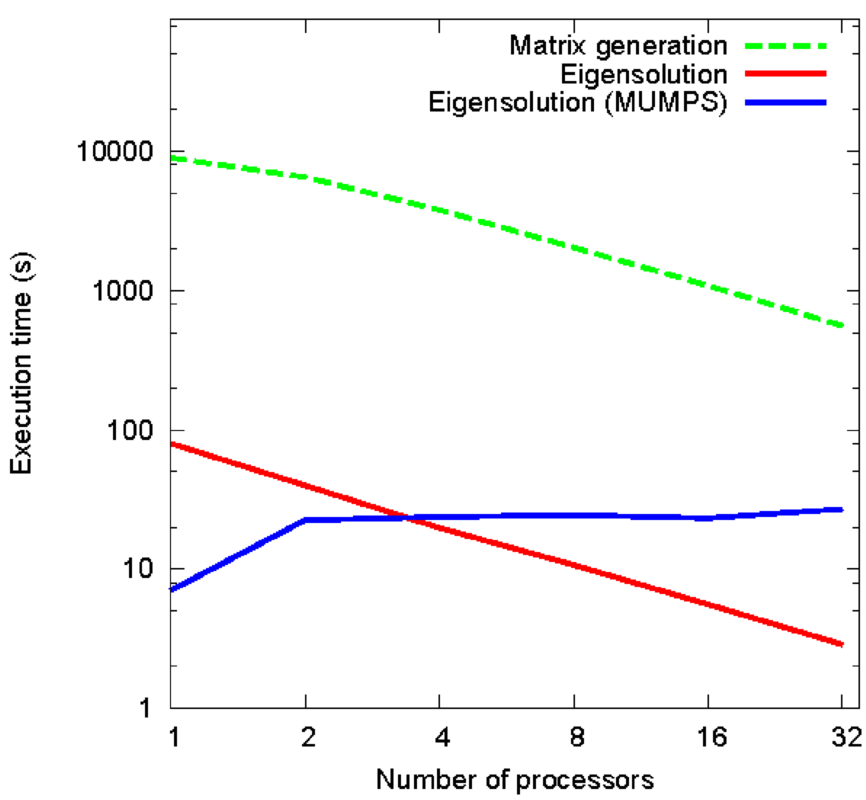
Execution times for the matrix generation and eigensolution phases on jacquard; five largest eigenvalues and corresponding eigenvectors.

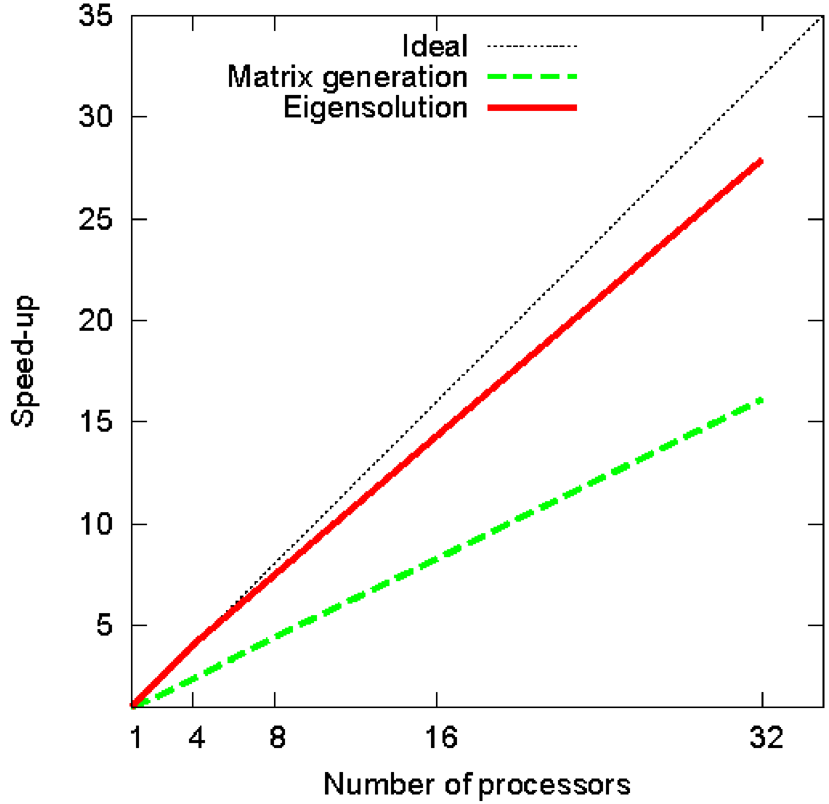
SLEPc: KS, JD and shift-and-invert

m	Krylov-Schur			Jacobi-Davidson		
	k	its	time	*k*	its	time
4K	48	230	27	48	68	14
8K	96	145	103	48	79	44
16K	192	119	789	48	89	181

- Both KS and JD fail to compute the required solutions in a reasonable time for large test cases
- Alternative: $(A - \varpi\, \mathrm{I})^{-1}x = (\lambda - \varpi)^{-1}\, x$

SLEPc: *times* and *speedup* on odin





Execution time and speed-up for the matrix generation and eigensolution stages with SLEPc corresponding to the 128K test case on odin.

Conclusions

- Both ScaLAPACK's (*pdsyevx*) and SLEPc (*Krylov-Schur and interface to PRIMME*) showed good scalability for the number of processors used, and the number of eigenvalues requested
- A direct method becomes more costly as the problem size increases, greatly surpassing the (already costly) generation of the matrix.
- Iterative methods can resolve multiplicities well and in the present application become the method of choice.

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