

Métodos iterativos para a resolução de equações integrais



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Análise Numérica

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75 Years of World-Class Science
1931-2006

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Aim



- In this work we consider the numerical solution of a radiative transfer equation for modeling the emission of photons in stellar atmospheres. **APPLICATION**
- Mathematically, the problem is formulated in terms of a weakly singular Fredholm integral equation defined on a Banach space. **MATHEMATICS**
- Computational approaches to solve the problem are discussed, using direct and iterative strategies that are implemented in open source packages. **COMPUTATIONS**

Outline



- Description of the astrophysics problem
- Numerical approach
 - Projection method: Kantorovich
 - Matrix formulation
 - Approximate solution:
 - iterative refinement methods
 - state-of-the-art numerical linear algebra algorithms
 - open source libraries
- Numerical results
- Conclusions

Description of the astrophysics problem



- Solve radiative transfer equation in stellar atmospheres

$$T\varphi = z\varphi + f \quad \text{Fredholm integral equation 2nd kind}$$

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

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

- τ is the optical depth of a stellar atmosphere
- τ^* optical thickness of the atmosphere
- z is on the resolvent set of T
- $f \in L^1(I)$ is the source term

Description of the astrophysics problem



- g is the kernel defined by $g(\tau) := \frac{\varpi}{2} E_1(\tau)$, $0 < \tau \leq \tau^*$
 - $\varpi \in]0, 1[$ is the albedo and

- E_1 is the first exponential-integral function and it belongs to the family

$$E_\nu(\tau) := \int_1^\infty \frac{\exp(-\tau\mu)}{\mu^\nu} d\mu, \tau > 0, \nu \geq 1$$

$$E'_{\nu+1}(\tau) = -E_\nu(\tau); E_\nu(0) = \frac{1}{\nu-1}, \nu > 1$$

- g is weakly singular in the sense that

$$\lim_{\tau \rightarrow 0^+} g(\tau) = +\infty; g \in C^0([0, \tau^*]) \cap X; \sup_{\tau \in [0, \tau^*]} \int_0^{\tau^*} g(|\tau - \tau'|) d\tau' < \infty$$

$g(\tau) > 0$ for all $\tau \in]0, \tau^*]$; g decreasing function on $]0, \tau^*]$

Projection method: Kantorovich

- Approximate $T\varphi = z\varphi + f$ by $T_n\varphi_n = z\varphi_n + f$

- consider a grid $0 = \tau_{n,0} < \tau_{n,1} < \dots < \tau_{n,n-1} < \tau_{n,n} = \tau^*$
 - define

$$X_n = \text{span} \{e_{n,j}, j = 1, \dots, n\}, e_{n,j} \in X$$

- Let π_n be the projection op. $\pi_n x = \sum_{j=1}^n \langle x, e_{n,j}^* \rangle e_{n,j}$
- $T_n x = \pi_n T x = \sum_{j=1}^n \langle x, T^* e_{n,j}^* \rangle e_{n,j}$
- where $e_{n,j}^*$ is the adjoint basis of $e_{n,j}$ in X^*

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Matrix formulation

- The solution of the approximate problem

$$T_n\varphi_n = z\varphi_n + f$$
- leads to the solution of a linear system with n eq's and n unknowns

$$(A_n - zI_n)x_n = b_n$$

- A_n is the restriction of T_n to X_n : $A_n = (\langle e_{n,j}, T^* e_{n,i}^* \rangle)_{i,j=1}^n$
 - $b_n = (\langle f, T^* e_{n,i}^* \rangle)_{i=1}^n$
 - $x_n = (\langle \varphi_n, T^* e_{n,i}^* \rangle)_{i=1}^n$

- we recover φ_n from x_n by $\varphi_n = \frac{1}{z} \left(\sum_{j=1}^n x_n(j) e_{n,j} - f \right)$

Error estimates

for n large enough:

$$\frac{\|\varphi - \varphi_n\|_1}{\|\varphi\|_1} \leq \frac{8c_0(z)}{q_n} \int_0^{h_n} g(\tau) d\tau$$

$$\exists n_0 : c_0(z) = \sup_{n > n_0} \|R_n(z)\|_1$$

h_n max. amplit. of subintervals,

μ_n min. amplit. of subintervals

$$q_n = \frac{\mu_n}{h_n}$$

Error estimates

for n large enough:

$$\frac{\|\varphi - \varphi_n\|_1}{\|\varphi\|_1} \leq c(1 - E_2(h_n)) = O(-h_n \ln h_n)$$

$$c \leq \frac{10}{q} \left(1 + \frac{1}{q} \right) \| (T - I)^{-1} \|_1$$

$$q = \inf_{grid} \frac{\min \{h_{n,i} : i = 1, \dots, n\}}{h_n}$$

$$d_{n,i,j} = |\tau_{n,i} - \tau_{n,j}|; \quad h_{n,i} = d_{n,i,i-1}$$

h_n max. amplit. of subintervals

Matrix coefficients: A_n

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

$$A_n(i, j) = \frac{\sigma}{2h_{n,i}} \int_{\tau_{n,i-1}}^{\tau_{n,i}} \int_0^{\tau^*} E_1(|\tau - \tau'|) e_{n,j}(\tau') d\tau' d\tau$$

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

$$d_{n,i,j} = |\tau_{n,i} - \tau_{n,j}|, \quad i, j \in [0, n] \quad h_{n,j} = \tau_{n,j} - \tau_{n,j-1}, \quad j \in [1, n]$$

RHS coefficients

for $i \in [1, n]$

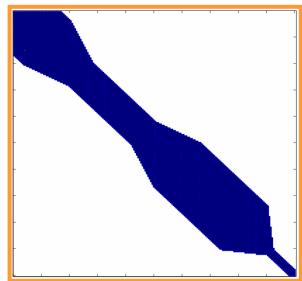
$$b_n(i) = \frac{\sigma}{2h_{n,i}} \int_{\tau_{n,i-1}}^{\tau_{n,i}} \int_0^{\tau^*} E_1(|\tau - \tau'|) f(\tau') d\tau' d\tau,$$

$$f(\tau) = \begin{cases} -1 & \text{if } 0 \leq \tau \leq \frac{\tau^*}{2} \\ 0 & \text{if } \frac{\tau^*}{2} < \tau \leq \tau^* \end{cases}$$

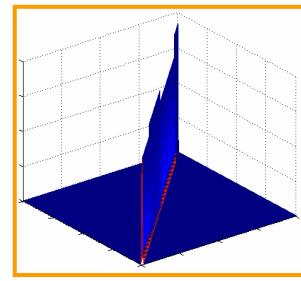
$$= \begin{cases} \frac{\sigma}{2h_{n,i}} \left[E_3 \left(\frac{\tau^*}{2} - \tau_{n,i} \right) - E_3 \left(\frac{\tau^*}{2} - \tau_{n,i-1} \right) \dots \right. \\ \left. \dots + E_3(\tau_{n,i}) - E_3(\tau_{n,i-1}) - 2h_{n,i} \right], & \tau_{n,i} \leq \frac{\tau^*}{2} \\ \frac{\sigma}{2h_{n,i}} \left[E_3 \left(\tau_{n,i} - \frac{\tau^*}{2} \right) - E_3 \left(\tau_{n,i-1} - \frac{\tau^*}{2} \right) \dots \right. \\ \left. \dots - E_3(\tau_{n,i}) + E_3(\tau_{n,i-1}) \right], & \tau_{n,i} > \frac{\tau^*}{2} \end{cases}$$

Typical coefficient matrix

$$A_n - zI_n, \quad z = 1$$



band and sparse matrix



strong decay in
magnitude from the
diagonal

Approximate solution

- How to solve $T_n \varphi_n = z \varphi_n + f$ when the associated coefficient matrix $A_n - zI_n$ has large dimension?
- one can use:
 - direct methods,
 - preconditioned nonstationary iterative methods, or
 - iterative refinement method (defect correction):

$$\begin{cases} & \text{given } x^{(0)} \\ x^{(k+1)} = x^{(k)} - (T - zI)^{-1} (Tx^{(k)} - zx^{(k)} - f) \end{cases}$$

- sequential or parallel computations

Iterative refinement methods

- Jacobian $(T - zI)^{-1}$ can be approximated by

– scheme A (**Atkinson**'s algorithm): $R_n(z) = (T_n - zI)^{-1}$

– scheme B (**Brakhage**'s algorithm): $(T(T_n - zI)^{-1} - I)/z$

– scheme C (**Ahues** algorithm): $((T_n - zI)^{-1} T - I)/z$

Iterative refinement methods: error estimates

for n large enough:
$$\frac{\|\varphi - x^{(k)}\|_1}{\|\varphi\|_1} \leq \left(\frac{c_1(z)}{q_n} \int_0^{h_n} g(\tau) d\tau \right)^{k+1}$$

$$\begin{aligned} \exists n_0 : \quad c_0(z) &= \sup_{n>n_0} \|R_n(z)\|_1, \\ c_1(z) &= 8c_0(z) \max\{1, \|T\|_1 / z\} \end{aligned}$$

h_n max. amplit. of subintervals,

μ_n min. amplit. of subintervals, $q_n = \mu_n / h_n$

Iterative refinement methods: error estimates

for n large enough:

$$\begin{aligned}
 \frac{\|\varphi - x^{(k)}\|_1}{\|\varphi\|_1} &\leq \left\| [R_n(z)(T - T_n)]^{k+1} \right\| \quad \text{scheme A} \\
 \dots &\leq \left\| \left[\frac{1}{z} R_n(z)(T - T_n) T \right]^{k+1} \right\| \quad \text{scheme B} \\
 \dots &\leq \left\| \left[\frac{1}{z} T R_n(z)(T - T_n) \right]^{k+1} \right\| \quad \text{scheme C}
 \end{aligned}$$

Iterative refinement methods

Scheme A:

$$\begin{cases} x^{(0)} = \varphi_n = R_n(z)f \\ x^{(k+1)} = x^{(0)} + R_n(z)(T_n x^{(k)} - T x^{(k)}) \quad k \geq 0 \end{cases}$$

Scheme B:

$$\begin{cases} x^{(0)} = \frac{1}{z}(R_n(z)T - I)f \\ x^{(k+1)} = x^{(0)} + \frac{1}{z}(R_n(z)T - I)(T_n x^{(k)} - T x^{(k)}) \quad k \geq 0 \end{cases}$$

Scheme C:

$$\begin{cases} x^{(0)} = \frac{1}{z}(T R_n(z) - I)f \\ x^{(k+1)} = x^{(0)} + \frac{1}{z}(T R_n(z) - I)(T_n x^{(k)} - T x^{(k)}) \quad k \geq 0 \end{cases}$$

Iterative refinement methods

- In practice T is not used. The problem is restricted to X_m , $m \gg n$, considering a finer projection discretization of T , T_m

- T_m restricted to X_m :
$$A_m = \left(\langle e_{m,j}, T^* e_{m,i}^* \rangle \right)_{i,j=1}^{m,m} \quad (m \times m)$$

- T_m restricted to X_n :
$$C = \left(\langle e_{m,j}, T^* e_{n,i}^* \rangle \right)_{i,j=1}^{n,m} \quad (n \times m)$$

- T_n restricted to X_m :
$$D = \left(\langle e_{n,j}, T^* e_{m,i}^* \rangle \right)_{i,j=1}^{m,n} \quad (m \times n)$$

Matrix coefficients: A_m , C and D

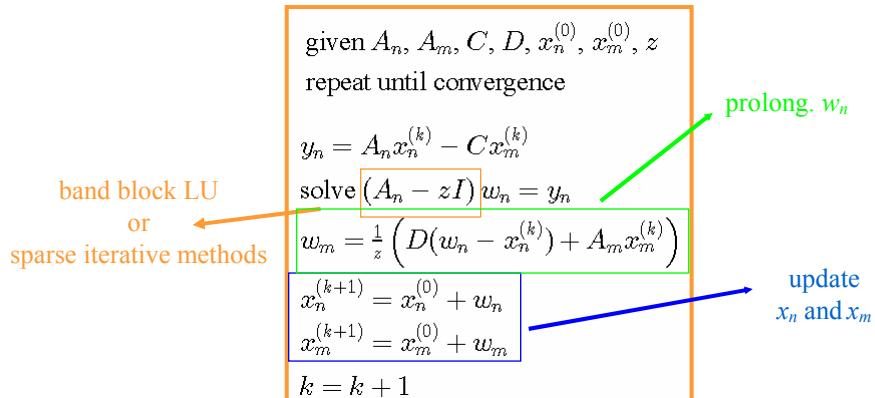
- Matrix A_m computed similarly to A_n
- We can compute matrices C and D :
 - through the integral formulation (similar to A_n and A_m)
 - or by doing some matrix computations using A_m

$$C = RA_m, \quad R(i, k) = \begin{cases} \frac{h_{m,k}}{h_{n,i}} & r \times (i-1) + 1 \leq k \leq r \times i \\ 0 & otherwise \end{cases}$$

$$D = A_m P, \quad P(k, j) = \begin{cases} 1 & r \times (j-1) + 1 \leq k \leq r \times j \\ 0 & otherwise \end{cases}$$

$r = \frac{m}{n}$

Atkinson's scheme



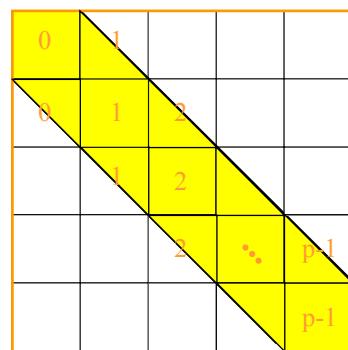
Problem specification

- grid τ^* : nonuniform grid (4 zones)
- parameters: $z = 1$, $\varpi = 0.75$, tol : $\varepsilon \leq 10^{-7}$ and $\varepsilon \leq 10^{-12}$
- data:
 - sparse and band structures
- machine:
 - PIV 2.4 GHz CPU with 256 MB RAM.
- software:
 - F77 & F95, LAPACK, BLAS

- Iterative refinement formulæ are competitive with the nonstationary iterative methods (based on Krylov subspaces) applied directly to the large linear system.
- For dense matrix discretizations all three iterative refinement schemes are faster than Krylov methods and than LU factorization even for small values of m .
- In the sparse case, for which Krylov methods are very well suited, iterative refinement execution times are comparable or even better in some cases (lower residual tolerances).
- And what about parallel computations?

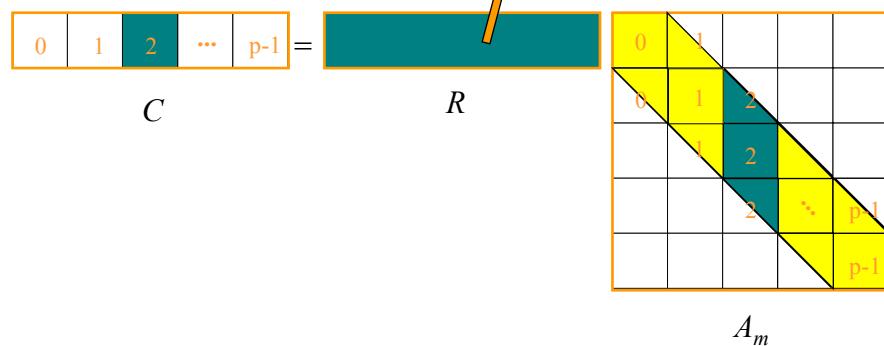
Data distribution

- Distributed memory environment with p processors:
 $p=0, \dots, p-1$



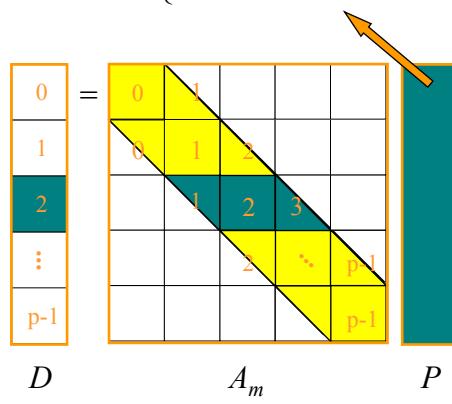
Matrix coefficients: C

$$C = RA_m, \quad R(i, k) = \begin{cases} \frac{h_{m,k}}{h_{n,i}} & r \times (i-1) + 1 \leq k \leq r \times i \\ 0 & \text{otherwise} \end{cases}$$



Matrix coefficients: D

$$D = A_m P, \quad P(k, j) = \begin{cases} 1 & r \times (j-1) + 1 \leq k \leq r \times j \\ 0 & \text{otherwise} \end{cases}$$



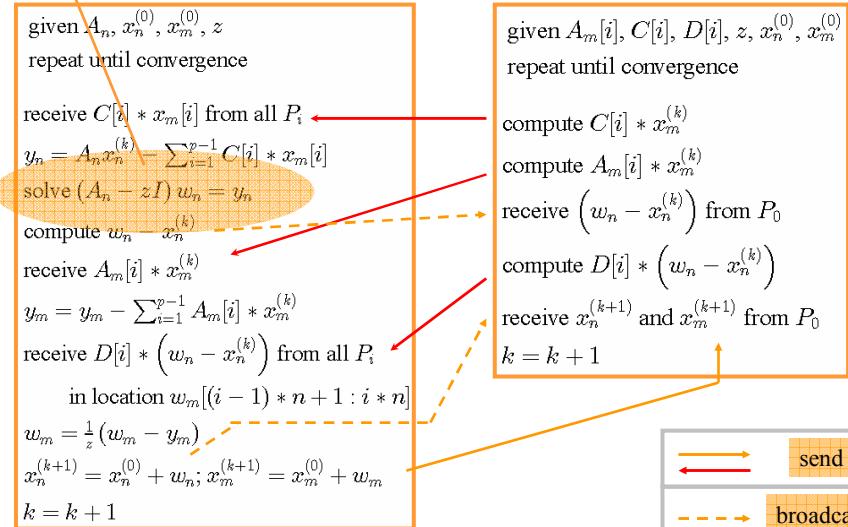
Matrix coefficients: D

$$D(i, j) = \frac{\varpi}{2h_{m,i}} \int_{\tau_{m,i-1}}^{\tau_{m,i}} \int_{\tau_{n,j-1}}^{\tau_{n,j+1}} E_1(|\tau - \tau'|) d\tau' d\tau$$

$$= \begin{cases} \frac{\varpi}{2h_{m,i}} [-E_3(\tau_{n,j} - \tau_{m,i}) + E_3(\tau_{n,j} - \tau_{m,i-1}) + E_3(\tau_{n,j-1} - \tau_{m,i}) - \\ - E_3(\tau_{n,j-1} - \tau_{m,i-1})] & , \quad \tau_{m,i-1} \leq \tau_{m,i} \leq \tau_{n,j-1} \leq \tau_{n,j} \\ \frac{\varpi}{2h_{m,i}} [-E_3(\tau_{m,i} - \tau_{n,j}) + E_3(\tau_{m,i-1} - \tau_{n,j}) + E_3(\tau_{m,i} - \tau_{n,j-1}) + \\ - E_3(\tau_{m,i-1} - \tau_{n,j-1})] & , \quad \tau_{n,j-1} \leq \tau_{n,j} \leq \tau_{m,i-1} \leq \tau_{m,i} \\ \varpi \left[1 + \frac{1}{2h_{m,i}} (-E_3(\tau_{n,j} - \tau_{m,i}) + E_3(\tau_{n,j} - \tau_{m,i-1}) + E_3(\tau_{m,i} - \tau_{n,j-1}) - \\ - E_3(\tau_{m,i-1} - \tau_{n,j-1})) \right] & , \quad \tau_{n,j-1} \leq \tau_{m,i-1} \leq \tau_{m,i} \leq \tau_{n,j} \end{cases}$$

may lead to scalability problems
for large number of processors

Atkinson's parallel scheme



Problem specification and computer environment

- grid τ^* : nonuniform grid (4 zones)
- parameters: $z = 1$, $\varpi = 0.75$, tol : $\varepsilon \leq 10^{-12}$
- Machine located at FEUP ^(out of service):
 - Beowulf cluster: 20 PIII 450 MHz processors (128 Mb RAM) connected via fast Ethernet switch (100 Mpbs)
- software:
 - MPI, F77 & F95, LAPACK, SPARSEKIT2

Nb. of iterations and elapsed times for the 3 iterative refinement methods

- $m = 10000, n = 1000$

p	scheme A	scheme B	scheme C
1	43 iterations	3472.7	3472.4
2		1749.4	1749.0
4		885.0	884.4
5		714.1	713.6
10		375.3	375.1

- $m = 100000, n = 5000$

20	14859.7	14855.0	14854.2
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*Speedup and efficiency
for the 3 iterative refinement methods*

- $m = 10000, n = 1000$

$$S_p = \frac{t_1}{t_p}; \quad E_p = \frac{S_p}{p}; \quad t_p = \text{elapsed time using } p \text{ processors}$$

p	schemes A, B and C	
	S_p	E_p
1	1	1.00
2	1.99	0.99
4	3.93	0.98
5	4.86	0.97
10	9.26	0.93

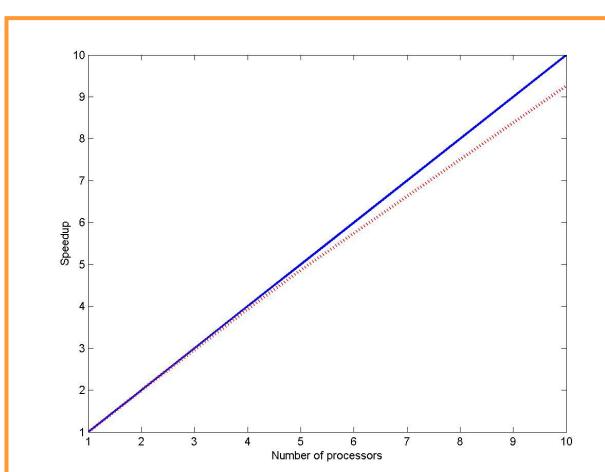
*Speedup up to 10 processors
for the 3 iterative refinement methods*

t_p = elapsed time using p processors

$$S_p = \frac{t_1}{t_p}$$

$$m = 10000$$

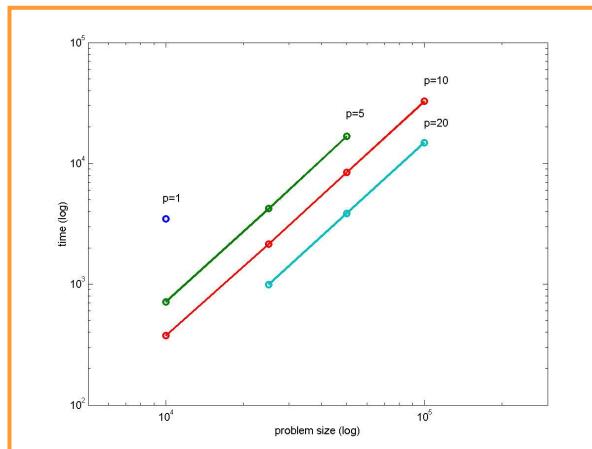
$$\frac{m}{n} = 10$$



- Isoefficiency or isogranularity (ScaLAPACK sense)
 - a constant memory use per node allows efficiency to be maintained

time for several size problems using up to 20 processors

$$\frac{m}{n} = 20$$



Solving the problem in the m-D space

- We can solve $T_m \varphi_m = z \varphi_m + f$ for the finer grid approximated matricial problem $A_m - zI_m = b_m$
- Our goal is to experiment with robust and portable algorithm implementations from the:



ACTS Collection - Advanced CompuTational Software

- LBNL and DOE
- Direct methods: SuperLU
- Preconditioned nonstationary iterative methods: PETSc

Problem specification

- grid τ^* : nonuniform grid (4 zones)
- parameters: $z = 1$, $\varpi = 0.75$ and $\varpi = 0.9$; tol : $\varepsilon \leq 10^{-12}$
- machines located at LBNL/NERSC
 - SGI Altix 350: 32 64-bit 1.4 GHz Intel Itanium-2 processors, with 192 GBytes of shared memory
 - AMD Opteron Cluster: 356 dual-processor nodes, 2.2 GHz/node, 6 GB/node, interconnected with a high-speed InfiniBand network
 - IBM SP: 380 compute nodes with 16 Power 3+ processors/node, 16 GB memory/node
- machine located at IRIC.UP
 - AMD Opteron Cluster: 24 64-bit dual-processor nodes, 2.4 Ghz/node, 4 GB/node, interconnected with a Gigabit Ethernet
- software:
 - MPI, F77 & F95, LAPACK, SPARSEKIT2, SuperLU, PETSc

Normalized times for the generation phase and system solution for various matrix sizes (m), on the SGI Altix and using SuperLU

$\varpi = 0.75$	generation		solution
	m		
1000	3.26E+03	6.95E+01	1.00E+00
2000	2.12E+04	1.65E+02	3.00E+00
4000	9.71E+04	3.59E+01	6.00E+00
8000	4.26E+05	7.51E+02	1.80E+01
16000	1.80E+06	1.54E+03	3.00E+01
32000	7.36E+06	3.12E+03	5.35E+01

$1.00E+00 = 1.953E-03$

Normalized times and nb. it. for various matrix sizes (m) on up to 32 processors (p), on the Opteron cluster and using PETSc

a constant memory use per node allows efficiency to be maintained

$\varpi = 0.75$		generation	GMRES	BiCGStab
m	p		22 iterations	14 iterations
10000	1	5.40E+03	7.54E+00	7.95E+00
	2	2.67E+03	4.02E+00	4.58E+00
	4	1.39E+03	2.32E+00	2.56E+00
	8	6.90E+02	1.80E+00	1.97E+00
	16	3.51E+02	1.15E+00	1.25E+00
	32	1.79E+02	1.15E+00	1.36E+00
25000	4	8.41E+03	5.42E+00	5.61E+00
	8	4.28E+03	3.02E+00	3.15E+00
	16	2.16E+03	2.05E+00	1.83E+00
	32	1.07E+03	1.00E+00	1.15E+00
50000	16	8.57E+03	3.14E+00	3.20E+00
	32	4.24E+03	1.53E+00	1.86E+00
				$1.00E+00 = 5.9E-02$

Normalized times and nb. it. for various matrix sizes (m) on up to 32 processors (p) on the Opteron cluster

$\varpi = 0.90$		$\varpi = 0.75$	generation	22	GMRES	14	BiCGStab
m	p			24 iterations		37 iterations	
10000	1	2.83E+03	6.14E+00		6.99E+00		
	2	1.36E+03	3.62E+00		4.12E+00		
	4	7.20E+02	2.20E+00		2.31E+00		
	8	3.59E+02	1.67E+00		1.76E+00		
	16	1.80E+02	1.11E+00		1.30E+00		
	32	9.19E+01	1.02E+00		1.00E+00		
25000	4	2.83E+03	4.72E+00		5.37E+00		
	8	2.22E+03	2.96E+00		3.39E+00		
	16	1.11E+03	1.78E+00		2.11E+00		
	32	5.55E+02	1.33E+00		1.46E+00		
50000	16	4.36E+03	2.82E+00		3.14E+00		
	32	2.21E+03	2.15E+00		2.05E+00		
							$1.00E+00 = 1.14E-01$

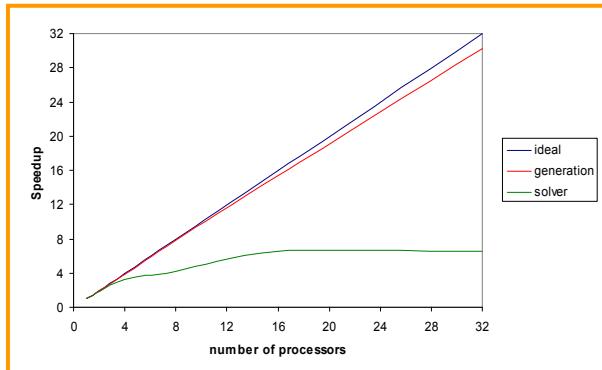
1.5x-2.5x smaller

Speedup up to 32 processors on the Opteron cluster

t_p = elapsed time using p processors

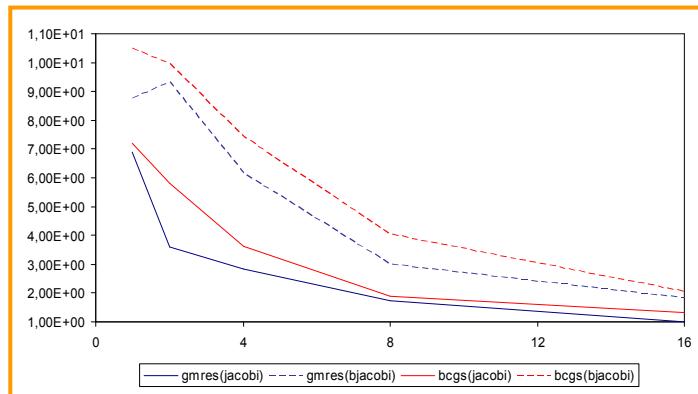
$$S_p = \frac{t_1}{t_p}$$

$m = 10000$



Normalized times for Jacobi and block Jacobi preconditioners on the Opteron cluster

$m = 50000$



Parallel IRM vs. Parallel preconditioned GMRES



- Compared to Iterative Refinement Techniques, the approach using parallel nonstationary iterative methods (GMRES, BiCGstab from PETSc), and for $m=50000$ and $p=5$
 - leads to 40% savings in time in the generation phase
 - reduces the number of communications required for mapping the coarse problem into the fine one
 - up to 5x for Atkinson and
 - up to 4x for Brakhage and Ahues' schemes
- To improve the performance of IRM:
 - parallelize the moderate size dimensional system (n -D linear systems)
 - explore the performance of 32 bit floating point arithmetic to obtain 64 bit accuracy => mixed-precision iterative refinement

Conclusions



- We discussed the numerical solution of a radiative transfer equation for modelling the emission of photons in stellar atmospheres.
- A good knowledge of the:
 - mathematics of the problem,
 - numerical methods, as well as,
 - computational aspects,were crucial for the implementation of an efficient and reliable solution.
- The parallelization of the generation phase greatly reduces the computation time and enables the solution of large dimensional problems.
- The selection of appropriate linear solvers is important for delivering performance and portability. The use of state-of-the-art linear algebra building blocks can ensure this task.
- **Further work:** using iterative refinement techniques and developing new algorithms for spectral computations

Main references

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