

Iterative Performance of Monte Carlo Linear Solver Methods

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Outline

- Motivations

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- Standard Monte Carlo vs. Monte Carlo Synthetic Acceleration (MCSA)

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- Choice of the preconditioner

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- Choice of the preconditioner
- Convergence conditions
- Numerical results

Motivations

Goal:

- development of reliable algorithms to solve highly dimensional (towards exascale) sparse linear systems in parallel

Issues:

- occurrence of **faults** (abnormal operating conditions of the computing system which cause a wrong answer)
 - hard faults
 - soft faults

[M. Hoemmen and M.A. Heroux, 2011; G. Bronevetsky and B.R. de Supinski, 2008; P. Prata and J.B. Silva, 1999]

Motivations

Resilience: ability to compute a correct output in presence of faults

Different approaches to tackle the problem:

- adaptation of Krylov subspace methods (CG, GMRES, Bi-CGSTab, ...) to fault tolerance by recover-restart strategies
- abandonment of deterministic paradigm in favor of stochastic approaches

[E. Agullo, L. Giraud, A. Guernouche, J. Roman and M. Zounon, 2013]

Monte Carlo Linear Solvers

Mathematical setting

Let us consider a sparse linear system

$$Ax = \mathbf{b}, \quad (1)$$

where $A \in \mathbb{R}^{n \times n}$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^n$.

With left preconditioning (1) becomes

$$P^{-1}Ax = P^{-1}\mathbf{b}, \quad P \in \mathbb{R}^{n \times n}. \quad (2)$$

(2) can be reinterpreted as a fixed point scheme

$$\mathbf{x} = H\mathbf{x} + \mathbf{f}, \quad H = I - P^{-1}A, \quad \mathbf{f} = P^{-1}\mathbf{b}. \quad (3)$$

Assuming $\rho(H) < 1$, (3) generates a sequence of approximate solutions $\{\mathbf{x}_k\}_{k=0}^{\infty}$ which converges to the exact solution of (1).

Monte Carlo Linear Solvers

Mathematical setting

The solution to (3) can be written in terms of a power series in H (Neumann series):

$$\mathbf{x} = \sum_{\ell=0}^{\infty} H^{\ell} \mathbf{f}.$$

By restricting the attention to a single component of \mathbf{x} we have

$$x_i = \sum_{\ell=0}^{\infty} \sum_{k_1=1}^n \sum_{k_2=1}^n \cdots \sum_{k_{\ell}=1}^n H_{k_0, k_1} H_{k_1, k_2} \cdots H_{k_{\ell-1}, k_{\ell}} f_{k_{\ell}}. \quad (4)$$

(4) can be reinterpreted as the **sampling of an estimator defined on a random walk**.

Monte Carlo Linear Solvers

Mathematical setting: Forward (Direct) Method

Goal: evaluate a functional such as

$$J(\mathbf{x}) = \langle \mathbf{h}, \mathbf{x} \rangle = \sum_{i=1}^n h_i x_i, \quad \mathbf{h} \in \mathbb{R}^n.$$

Approach: define random walks to evaluate J .

Consider a random walk whose state space S is the set of indices of the forcing term \mathbf{f} :

$$S = \{1, 2, \dots, n\} \subset \mathbb{N}.$$

[N. Metropolis and S. Ulam, 1949; G. E. Forsythe and A. Leibler, 1950; W. R. Wasow, 1952; J. H. Halton, 1962]

Monte Carlo Linear Solvers

Mathematical setting: Forward (Direct) Method

Initial probability: pick k_0 as initial step of the random walk:

$$\tilde{p}(k_0 = i) = \tilde{p}_{k_0} = \frac{|h_i|}{\sum_{i=1}^n |h_i|}.$$

Possible choices for the transition probability:

$$p(:, i) : S \rightarrow [0, 1] \quad \forall i \in S$$

$$p(k_i = j | k_{i-1} = i) = P_{i,j} = \frac{|H_{i,j}|}{\sum_{i=1}^n |H_{i,j}|} \quad \text{weighted}$$

$$P_{i,j} = \begin{cases} 0 & \text{if } H_{i,j} = 0 \\ \frac{1}{\#(\text{non-zeros in the row})} & \text{if } H_{i,j} \neq 0 \end{cases} \quad \text{uniform}$$

Monte Carlo Linear Solvers

Mathematical setting: Forward (Direct) Method

A related sequence of weights is defined by

$$w_{i,j} = \frac{H_{i,j}}{P_{i,j}}$$

in order to build an auxiliary sequence

$$W_0 = \frac{h_{k_0}}{\tilde{p}_{k_0}}, \quad W_i = W_{i-1} w_{k_{i-1}, k_i} \quad k_{i-1}, k_i \in S.$$

This allows us to define a random variable $X(\cdot) : \Pi \rightarrow \mathbb{R}$.

Π = set of realizations of a random walk γ defined on S :

$$X(\nu) = \sum_{\ell=0}^{\infty} W_{\ell} f_{k_{\ell}}, \quad \nu = \text{permutation of } \gamma$$

Monte Carlo Linear Solvers

Mathematical setting: Forward (Direct) Method

Define the expected value of $X(\cdot)$:

$$E[X] = \sum_{\nu} P_{\nu} X(\nu) \quad (P_{\nu} = \text{probability of the permutation } \nu).$$

It can be proved that

$$E[W_{\ell} f_{k_{\ell}}] = \langle \mathbf{h}, H^{\ell} \mathbf{f} \rangle$$

and consequently

$$E \left[\sum_{\ell=0}^{\infty} W_{\ell} f_{k_{\ell}} \right] = \langle \mathbf{h}, \mathbf{x} \rangle .$$

Monte Carlo Linear Solvers

Mathematical setting: Forward (Direct) Method

If \mathbf{h} is a vector of the standard basis: $\mathbf{h} = \mathbf{e}_j$

$$\tilde{p}(K_0 = i) = \delta_{i,j}, \quad i, j = 1, \dots, n$$

and the expected value assumes the following form:

$$E \left[\sum_{\ell=0}^{\infty} W_{\ell} f_{\mathbf{k}_{\ell}} \right] = x_i = \sum_{\ell=0}^{\infty} \sum_{\mathbf{k}_1=1}^n \sum_{\mathbf{k}_2=1}^n \cdots \sum_{\mathbf{k}_{\ell}=1}^n P_{\mathbf{k}_0, \mathbf{k}_1} P_{\mathbf{k}_1, \mathbf{k}_2} \cdots P_{\mathbf{k}_{\ell-1}, \mathbf{k}_{\ell}} w_{\mathbf{k}_0, \mathbf{k}_1} w_{\mathbf{k}_1, \mathbf{k}_2} \cdots w_{\mathbf{k}_{\ell-1}, \mathbf{k}_{\ell}} f_{\mathbf{k}_{\ell}}. \quad (5)$$

Drawback: the estimator is defined entry-wise.

Monte Carlo Linear Solvers

Mathematical setting: Adjoint Method

Consider the adjoint linear system

$$(P^{-1}A)^T \mathbf{y} = \mathbf{d}.$$

With a fixed point approach, we get

$$\mathbf{y} = H^T \mathbf{y} + \mathbf{d}.$$

By picking $\mathbf{d} = \mathbf{e}_j$ we have

$$J^*(\mathbf{y}) := \langle \mathbf{y}, \mathbf{f} \rangle = \langle \mathbf{x}, \mathbf{e}_j \rangle = x_j, \quad j = 1, \dots, n.$$

Monte Carlo Linear Solvers

Mathematical setting: Adjoint Method

The initial probability and transition matrix may be defined as

$$\tilde{p}_{k0} = p(k_0 = i) = \frac{|f_i|}{\sum_{i=1}^n |f_i|}, \quad P_{i,j} = \frac{|H_{i,j}^T|}{\sum_{k=1}^n |H_{i,k}^T|} = \frac{|H_{j,i}|}{\sum_{k=1}^n |H_{k,i}|}.$$

Reintroduce weights as before:

$$w_{i,j} = \frac{H_{j,i}}{P_{i,j}} \Rightarrow W_0 = \text{sign}(f_i) \|\mathbf{f}\|_1, \quad W_j = W_{j-1} w_{k_{j-1}, k_j}, \quad k_{j-1}, k_j \in S.$$

Expected value of the estimator for the entire solution vector \mathbf{x} :

$$E \left[\sum_{\ell=0}^{\infty} W_{\ell} d_{k_{\ell}} \right] = \sum_{\ell=0}^{\infty} \sum_{k_1}^n \sum_{k_2}^n \cdots \sum_{k_{\ell}}^n f_{k_0} P_{k_0, k_1} P_{k_1, k_2} \cdots P_{k_{\ell-1}, k_{\ell}} W_{k_0, k_1} \cdots W_{k_{\ell-1}, k_{\ell}} \delta_{k_{\ell}, j}. \quad (6)$$

Monte Carlo Linear Solvers

Statistical constraints for convergence

Expected value and variance of the estimator must be finite to apply the Central Limit Theorem.

$$\text{Forward Method: } (H^*)_{i,j} = \frac{(H_{i,j})^2}{P_{i,j}}$$

$$E\left[\sum_{\ell=0}^{\infty} W_{\ell} f_{\mathbf{k}_{\ell}}\right] < \infty \Leftrightarrow \rho(H) < 1$$

$$\text{Var}\left[\sum_{\ell=0}^{\infty} W_{\ell} f_{\mathbf{k}_{\ell}}\right] < \infty \Leftrightarrow \rho(H^*) < 1$$

$$\text{Adjoint Method: } (H^*)_{i,j} = \frac{(H_{j,i})^2}{P_{i,j}}$$

$$E\left[\sum_{\ell=0}^{\infty} W_{\ell} d_{\mathbf{k}_{\ell}}\right] < \infty \Leftrightarrow \rho(H) < 1$$

$$\text{Var}\left[\sum_{\ell=0}^{\infty} W_{\ell} d_{\mathbf{k}_{\ell}}\right] < \infty \Leftrightarrow \rho(H^*) < 1$$

[J. H. Halton, 1994; H. Ji, M. Mascagni and Y. Li, 2013]

Monte Carlo Linear Solvers

The choice of the transition probability

Theorem (H. Ji, M. Mascagni and Y. Li)

Let $H \in \mathbb{R}^{n \times n}$, where $\|H\|_\infty < 1$ for the Forward method and $\|H\|_1 < 1$ for the Adjoint method. Consider ν_k as the realization of a random walk γ truncated at the k -th step. Then, there always exists a transition matrix P such that $\text{Var}(X(\nu_k)) \rightarrow 0$ and $\text{Var}(\sum_\nu X(\nu_k))$ is bounded as $k \rightarrow \infty$.

Remark If the hypotheses hold, then $P_{i,j} = \frac{|H_{i,j}|}{\sum_{k=1}^n |H_{i,k}|}$ (Forward) or $P_{i,j} = \frac{|H_{i,j}^T|}{\sum_{k=1}^n |H_{i,k}^T|}$ (Adjoint) guarantee $\|H^*\|_\infty < 1$ or $\|H^*\|_1 < 1$ respectively.

Monte Carlo Linear Solvers

First approaches to a parallelization

First attempts to apply Monte Carlo as a linear solver considered the fixed point formulation of the original linear system.

- + embarrassingly parallelizable (ideally we could employ as many processes as the amount of histories)
- huge amount of time to compute a reasonably accurate solution

E.g. $\|r_0\| = \|\mathbf{b} - A\mathbf{x}_0\| \approx 1$ then $\frac{\|\mathbf{r}_k\|}{\|\mathbf{b}\|} < 10^{-m} \Rightarrow N_{histories} \approx 10^{2m}$
because of the Central Limit Theorem.

[S. Branford, C. Sahin, A. Thandavan, C. Weihrauch, V. N. Alexandrov and I. T. Dimov, 2008; P. Jakovits, I. Kromonov and S. R. Srirama, 2011]

Monte Carlo Linear Solvers

Monte Carlo Synthetic Acceleration (MCSA)

Data: $A, \mathbf{b}, H, \mathbf{f}, \mathbf{x}_0$

Result: \mathbf{x}_{num}

$\mathbf{x}^I = \mathbf{x}_0;$

while not reached convergence do

$$\mathbf{x}^{I+\frac{1}{2}} = H\mathbf{x}^I + \mathbf{f};$$

$$\mathbf{r}^{I+\frac{1}{2}} = \mathbf{b} - A\mathbf{x}^{I+\frac{1}{2}};$$

$$\delta\mathbf{x}^{I+\frac{1}{2}} = (I - H)^{-1}\mathbf{r}^{I+\frac{1}{2}};$$

"Solved" with Standard MC

$$\mathbf{x}^{I+1} = \mathbf{x}^{I+\frac{1}{2}} + \delta\mathbf{x}^{I+\frac{1}{2}};$$

end

$$\mathbf{x}_{num} = \mathbf{x}^{I+1}$$

[S. Slattery, 2013 (PhD Thesis); T. M. Evans, S. R. Slattery and P. P. H. Wilson, 2013]

Adaptivity for the number of random walks

Forward Method:

$$\theta_i \in \mathbb{R}$$

$$\theta_i = E \left[\sum_{l=0}^{\infty} W_l b_{k_l} \right]$$

$$\sigma_i = \sqrt{\text{Var}[\theta_i]}$$

$$\text{Find } \tilde{N}_i \quad \text{s.t.} \quad \frac{\sigma_i^{\tilde{N}_i}}{|\hat{x}_i|} < \varepsilon$$

$$i = 1, \dots, n$$

Adjoint Method:

$$\boldsymbol{\theta} \in \mathbb{R}^n$$

$$\boldsymbol{\theta}_i = E \left[\sum_{l=0}^{\infty} W_l d_{k_l} \delta_{k_l, i} \right]$$

$$\boldsymbol{\sigma}_i = \sqrt{\text{Var}[\boldsymbol{\theta}]_i}$$

$$\text{Find } \tilde{N} \quad \text{s.t.} \quad \frac{\|\boldsymbol{\sigma}^{\tilde{N}}\|_1}{\|\hat{\mathbf{x}}\|_1} < \varepsilon$$

$$i = 1, \dots, n$$

Applicable preconditioning techniques

Remark: explicit knowledge of H_{ij} is needed

In fact the entry P_{ij} of the transition matrix is defined in terms of H_{ij} (Forward method) or H_{ji} (Adjoint method).

This limits the viable choices of preconditioners:

- diagonal preconditioners
- block diagonal preconditioners
- sparse approximate inverse preconditioners (AINV)

Monte Carlo Linear Solvers

Examples

Strictly diagonally dominant matrices (s.d.d.) with diagonal preconditioning.

$A \in \mathbb{R}^{n \times n}$ s.d.d. by rows: $P = \text{diag}(A)$

$H = I - P^{-1}A$, $\|H\|_{\infty} < 1$ ($\Leftrightarrow \|H^*\|_{\infty} < 1$)

$A \in \mathbb{R}^{n \times n}$ s.d.d. by columns: $P = \text{diag}(A)$

$H = I - AP^{-1}$, $\|H\|_1 < 1$ ($\Leftrightarrow \|H^*\|_1 < 1$)

Strict diag. dominance	Forward Method	Adjoint method
by rows	converges	not guaranteed
by columns	not guaranteed	converges

Monte Carlo Linear Solvers

Examples

Other examples:

- A M -matrix $\Rightarrow \exists D$ diagonal s.t. AD is s.d.d.
- with preconditioner $P = \text{block_diag}(A)$:

$$\left\{ \sum_{\substack{j=1 \\ j \neq i}}^p \|A_{ii}^{-1} A_{ij}\|_{\infty} < 1. \quad \forall i = 1, \dots, p \right. \Rightarrow \text{Forward method with block Jacobi converges}$$

$$\left\{ \sum_{\substack{i=1 \\ i \neq j}}^p \|A_{ii}^{-1} A_{ij}\|_1 < 1. \quad \forall j = 1, \dots, p \right. \Rightarrow \text{Adjoint method with block Jacobi converges}$$

2D parabolic problems: test case 1

Give an open and bounded set $\Omega \subset \mathbb{R}^2$ s.t. $\Omega = (0, 2)^2 \setminus (1, 2)^2$

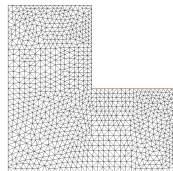
$$\begin{cases} \frac{\partial u}{\partial t} - \mu \Delta u + \beta(\mathbf{x}) \cdot \nabla u = 0, & \mathbf{x} \in \Omega, \quad t \in (0, T] \\ u(\mathbf{x}, 0) = u_0, & \mathbf{x} \in \Omega \\ u(\mathbf{x}, t) = 0, & \mathbf{x} \in \Gamma_D, \quad t \in (0, T] \\ \frac{\partial u}{\partial n} + \chi u = 0, & \mathbf{x} \in \Gamma_R, \quad t \in (0, T] \end{cases} \quad (7)$$

where $\mu = \frac{3}{200}$, $\chi = 3$, $\beta(\mathbf{x}) = [x, -y]^T$.

$\Gamma_R = \{\{x = 1\} \times (1, 2)\} \cup \{(1, 2) \times \{y = 1\}\}$, $\Gamma_D = \partial\Omega \setminus \Gamma_R$.

Discretization (FreeFem++ employed):

- Triangular FEM
- spatial discretization step $h_{\max} = 0.018$, 37,177 d.o.f.'s
- time discretization step $\Delta t = h_{\max}^2$



2D parabolic problems: test case 1

Preconditioning: sparse factorized AINV with drop tolerance $\tau = 0.05$. Code provided by courtesy by Miroslav Tuma.
[M. Benzi and M. Tuma, SISC, 1998]

Numerical setting:

- Adjoint MCSA employed as linear solver
- relative residual tolerance: $\varepsilon_1 = 10^{-7}$
- weighted transition probability
- maximal # steps per history: 10
- statistical error-based adaptive parameter: $\varepsilon_2 = 0.01$
- granularity of the adaptive approach: $n_{histories} = 100$
- simulations run on laptop

2D parabolic problems: test case 1

Stiffness matrix: A ($n = 37,177$), s.d.d. by rows and columns.

AINV preconditioner: M . Drop tolerance $\tau = 0.05$ for both factors.

Iteration matrix: $H = I - MA$.

Solution computed just for a generic time step.

- $\frac{\text{nnz}(H)}{\text{nnz}(A)} = 2.984$
- $\|H\|_1 = 0.597$ ($\rho(H) \approx 0.286$, $\rho(H^*) \approx 0.104$)
- # MCSA iterations: 8
- relative error = $2.71 \cdot 10^{-8}$
- # total random walks employed: 90,000

2D parabolic problems: test case 2

Give an open and bounded set $\Omega = (0, 1) \times (0, 1)$

$$\begin{cases} \frac{\partial u}{\partial t} - \mu \Delta u + \beta(\mathbf{x}) \cdot \nabla u = 0, & \mathbf{x} \in \Omega, \quad t \in (0, T] \\ u(\mathbf{x}, 0) = u_0, & \mathbf{x} \in \Omega \\ u(\mathbf{x}, t) = 0, & \mathbf{x} \in \partial\Omega, \quad t \in (0, T] \end{cases} \quad (8)$$

where $\mu = \frac{3}{200}$, $\beta(\mathbf{x}) = [2, \sin(x)]^T$.

Discretization (FreeFem++ employed):

- Triangular FEM
- spatial discretization step $h_{max} = 0.014$, 40,501 d.o.f.'s
- time discretization step $\Delta t = h_{max}^2$

2D parabolic problems: test case 2

Stiffness matrix: A ($n = 40,501$), s.d.d. by rows and columns.

AINV preconditioner: M . Drop tolerance $\tau = 0.05$ for both factors.

Iteration matrix: $H = I - MA$.

Solution computed just for a generic time step.

- $\frac{\text{nnz}(H)}{\text{nnz}(A)} = 3.106$
- $\|H\|_1 = 0.185 \quad (\rho(H) \approx 0.083, \rho(H^*) \approx 0.017)$
- # MCSA iterations: 6
- relative error = $5.148 \cdot 10^{-8}$
- # total random walks employed: 66,800

2D parabolic problems: test case 3

Give an open and bounded set $\Omega = (0, 1) \times (0, 1)$

$$\begin{cases} \frac{\partial u}{\partial t} - \mu \Delta u + \beta(\mathbf{x}) \cdot \nabla u = 0, & \mathbf{x} \in \Omega, \quad t \in (0, T] \\ u(\mathbf{x}, 0) = u_0, & \mathbf{x} \in \Omega \\ u(\mathbf{x}, t) = u_D(\mathbf{x}), & \mathbf{x} \in \partial\Omega, \quad t \in (0, T] \end{cases} \quad (9)$$

where $\mu = \frac{3}{200}$, $\beta(\mathbf{x}) = [2y(1 - x^2), -2x(1 - y^2)]^T$,
 $u_D = 0$ on $\{\{x = 0\} \times (0, 1)\}, \{(0, 1) \times \{y = 0\}\}, \{(0, 1) \times \{y = 1\}\}$.

Discretization (IFISS toolbox employed):

- Quadrilateral FEM
- spatial discretization step $h = 2^{-8} \Rightarrow 66,049$ d.o.f.'s
- time discretization step $\Delta t = h^2$

2D parabolic problems: test case 3

Stiffness matrix: A ($n = 66,049$). Not s.d.d.

AINV preconditioner: M . Drop tolerance $\tau = 0.05$ for both factors.

Iteration matrix: $H = I - MA$.

Solution computed just for a generic time step.

- $\frac{\text{nnz}(H)}{\text{nnz}(A)} = 4.736$
- $\|H\|_1 = 0.212$ ($\rho(H) \approx 0.171, \rho(H^*) \approx 0.032$)
- # MCSA iterations: 8
- relative error = $1.7153 \cdot 10^{-8}$
- # total random walks employed: 88,400

Conclusions and future developments

Conclusions

- MC solvers motivated by resilience
- hypotheses for convergence difficult to satisfy in general
- currently best results obtained using AINV

Future developments

- extension of the set of matrices for which MC solvers is guaranteed to converge a priori
- analysis of how $\rho(H)$ and $\rho(H^*)$ affect convergence
- refinement of the adaptive selection of histories

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Monte Carlo Linear Solvers

The choice of the transition probability

Theorem (H. Ji, M. Mascagni and Y. Li)

Let $H \in \mathbb{R}^{n \times n}$ with spectral radius $\rho(H) < 1$. Let $H^+ \in \mathbb{R}^{n \times n}$ where $H_{i,j}^+ = |H_{i,j}|$. Consider ν_k as the realization of a random walk γ truncated at the k -th step. If $\rho(H^+) > 1$, there does not exist a transition matrix P such that $\text{Var}(X(\nu_k))$ converges to zero as $k \rightarrow \infty$.

Numerical experiments

Simplified P_N equations

Steady-state, multigroup, one-dimensional, eigenvalue-form of Boltzmann transport equation:

$$\begin{aligned} \mu \frac{\partial \psi^g(x, \mu)}{\partial x} + \sigma^g(x) \psi^g(x, \mu) &= \sum_{g'=1}^{N_g} \int_{4\pi} \sigma_s^{gg'}(x, \hat{\Omega} \cdot \hat{\Omega}') \psi^{g'}(x, \Omega') d\Omega' + \\ &+ \frac{1}{k} \sum_{g'=1}^{N_g} \frac{\chi^g}{4\pi} \int_{4\pi} \nu \sigma_f^{g'}(x) \psi^{g'}(x, \Omega') d\Omega'. \end{aligned} \quad (10)$$

$\psi^g(x, \mu)$ = angular flux for group g

σ^g = total interaction cross section

$\sigma_s^{gg'}(x, \hat{\Omega} \cdot \hat{\Omega}')$ = scattering cross section from group $g' \rightarrow g$

Numerical experiments

Simplified P_N equations

- Legendre polynomial spectral discretization (P_N equations)
- consider just odd sets of P_N equations
- removing lower order gradient terms from each equation (SP_N equations)

$$-\nabla \cdot \mathbb{D}_n \nabla \mathbf{U}_n + \sum_{m=0}^{\frac{N+1}{2}} \mathbb{A}_{nm} \mathbf{U}_m = \frac{1}{k} \sum_{m=1}^{\frac{N+1}{2}} \mathbb{F}_{nm} \mathbf{U}_m, \quad n = 1, \dots, \frac{N+1}{2} \quad (11)$$

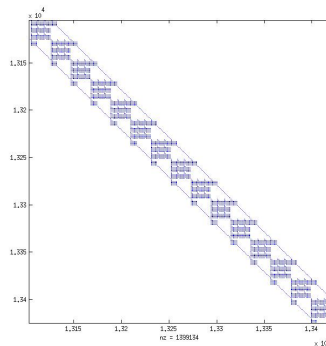
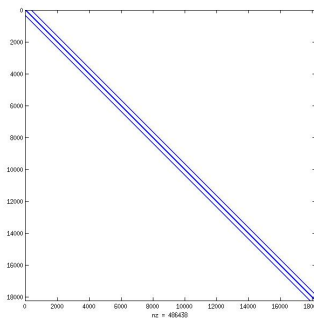
\mathbf{U}_m is a linear combination of moments.

- Discretized with Finite Volumes

Numerical experiments

Simplified P_N equations

Sparsity pattern and zoom on the structure of a SP_1 matrix



Numerical experiments

Simplified P_N equations

Properties of matrices:

- discretization of SP_1 equations
- all nonzero diagonal entries

Numerical treatment:

- block Jacobi preconditioning

Kind of matrix	size	nnz	Prec. block size	nnz after prec
SP_1 (a)	18,207	486,438	63	2,644,523
SP_1 (b)	19,941	998,631	69	1,774,786

[Matrices provided by courtesy by Thomas Evans, Steven Hamilton, Stuart Slattery, ORNL]

Numerical experiments

Simplified P_N equations

MCSA parameter setting:

- Adjoint method
- residual relative tolerance: $\varepsilon_1 = 10^{-7}$
- almost optimal transition probability
- maximal # steps per history: 10
- statistical error-based adaptive parameter: $\varepsilon_2 = 0.5$
- granularity of the adaptive approach: $n_{histories} = 1,000$
- simulations run in serial mode

Numerical experiments

Simplified P_N equations

matrix	$\rho(H)$	$\rho(H^*)$	relative err.	# iterations
SP_1 (a)	0.9779	0.9758	$9.97 \cdot 10^{-6}$	340
SP_1 (b)	0.9798	0.9439	$3.89 \cdot 10^{-5}$	209

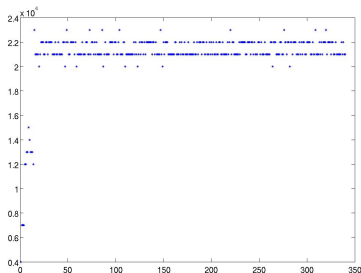


Figure 1 : # histories for (a) at each iteration.

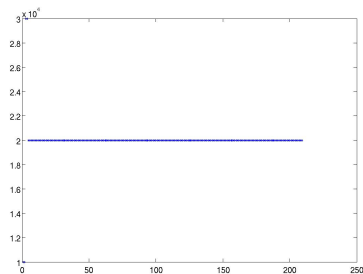


Figure 2 : # histories for (b) at each iteration.

Numerical experiments

Simplified SP_N equations

Issues raised for a general SP_N matrix:

- hard to find a block Jacobi preconditioner s.t. $\rho(H^*) < 1$ for every SP_N problem
- attempt to use Approximate Inverse preconditioners was not effective
 - for sparse preconditioners $\rho(H^*) < 1$ is not respected
- attempt to use ILU preconditioners was not effective
 - for ILU(0) we got $\rho(H^*) > 1$
 - massive fill-in with ILUT
- reordering and scaling did not facilitate the convergence requirements

Numerical experiments

Diagonally dominant matrices

Set of matrices obtained by a diagonal shift of matrices associated with SP_1 , SP_3 and SP_5 equations.

$$(A + sD), \quad s \in \mathbb{R}^+, \quad D = \text{diag}(A).$$

All the matrices have been turned into s.d.d. by columns.

Initial matrix	s	$\rho(H)$	$Forward - \rho(H^*)$	$Adjoint - \rho(H^*)$
SP_1 (a)	0.3	0.7597	0.7441	0.6983
SP_1 (b)	0.4	0.7046	1.1448	0.5680
SP_3	0.9	0.5869	0.4426	0.3727
SP_5	1.6	0.5477	0.3790	0.3431

Numerical experiments

Diagonally dominant matrices

$$(A + sD), \quad s \in \mathbb{R}^+, \quad D = \text{diag}(A).$$

matrix	nnz	s	relative err.	# iterations
SP_1 (a)	486,438	0.3	$6.277 \cdot 10^{-7}$	36
SP_1 (b)	998,631	0.4	$9.885 \cdot 10^{-7}$	21
SP_3	846,549	0.9	$5.919 \cdot 10^{-7}$	18
SP_5	1,399,134	1.6	$4.031 \cdot 10^{-7}$	19

Numerical experiments

Diagonal shift

Strict diagonally dominance is a sufficient condition for convergence but not necessary.

$$(A + sD), \quad s \in \mathbb{R}^+, \quad D = \text{diag}(A)$$

such that $\rho(H) < 1$ and $\rho(H^*) < 1$.

Initial matrix	s	$\rho(H)$	$Forward - \rho(H^*)$	$Adjoint - \rho(H^*)$
SP_1 (a)	0.2	0.8230	0.8733	0.8195
SP_1 (b)	0.2	0.8220	1.5582	0.7731
SP_3	0.3	0.8126	0.9459	0.7961
SP_5	0.7	0.8376	0.8865	0.8026

Numerical experiments

Diagonal shift

$$(A + sD), \quad s \in \mathbb{R}^+, \quad D = \text{diag}(A).$$

matrix	s	relative err.	# iterations
SP_1 (a)	0.2	$6.394 \cdot 10^{-7}$	48
SP_1 (b)	0.2	$2.59 \cdot 10^{-6}$	36
SP_3	0.3	$5.35 \cdot 10^{-7}$	45
SP_5	0.7	$4.21 \cdot 10^{-7}$	70