SAND2011-3115C

Generation of Accurate Benchmarks for Transport in Stochastic Media by Means of Dynamic Error Control

Shawn D. Pautz
Brian C. Franke
Sandia National Laboratories
Albuquerque, NM, U.S.

International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011)
Rio de Janeiro, Brazil
May 12, 2011

Outline

- Objectives
- Benchmark process with error control
- Results
- Conclusions

Objectives

The generation of benchmarks for transport in stochastic media is computationally intensive, so we want to reduce computer time where possible.

The nature of benchmarks requires good accuracy as well as assurances that it is good.

→ We want to measure and control errors for efficient computations

Additional motivation

Computational physics increasingly requires quantification of errors. This requires both good error estimates as well as ensemble calculations. The current work on stochastic benchmarks may have lessons for other analyses.

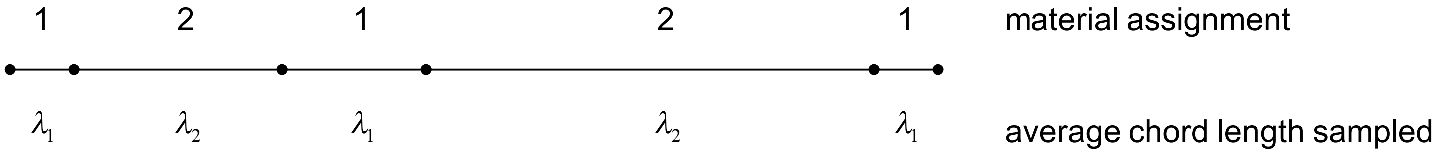
Sources of error

- Statistical (insufficient realizations)
- Discretization (space, angle, energy)
- Iterative

We assume the use of a verified code!

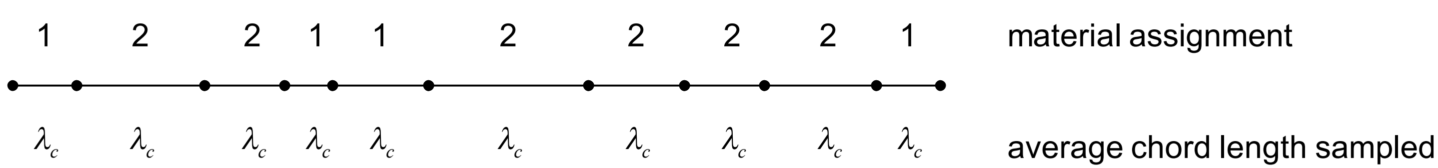
Common method of generating stochastic realizations in 1D

- We sample from two materials (1 and 2) with average chord lengths λ_1 and λ_2
- Randomly choose the material at the left boundary and the chord length based on that material
- Alternate between the two materials to choose chord lengths

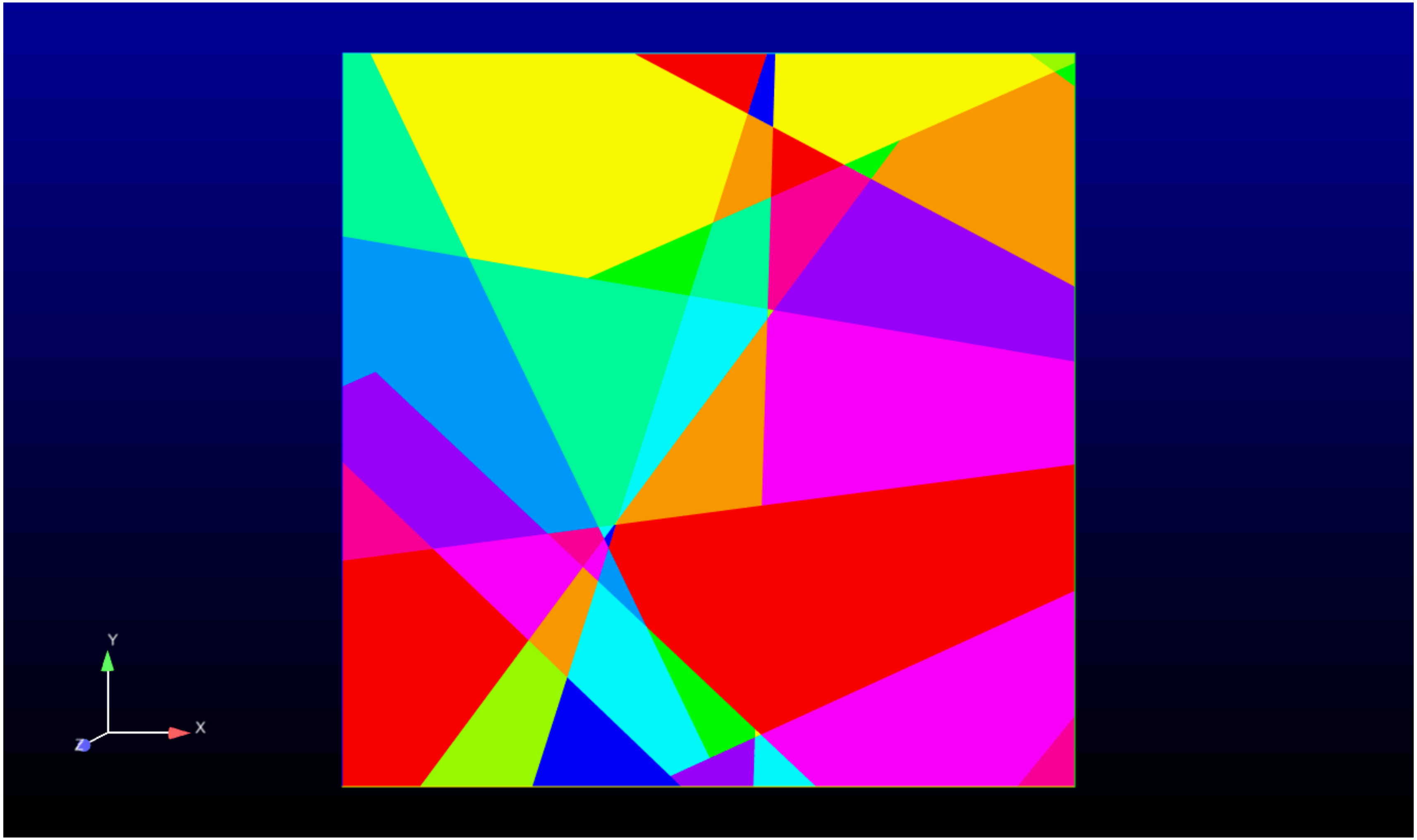


Alternative method of generating stochastic realizations in 1D

- Define effective combined material with average chord length $\lambda_c = \lambda_1 \lambda_2 / (\lambda_1 + \lambda_2)$
- Generate geometry as before using the single effective material
- Randomly assign materials 1 and 2 to each region in proportion to their abundance
- Motivation: separates geometry generation from material assignment and is extendable to multi-D



Example: 2D Markovian geometry



Sandia National Laboratories

Control of statistical error

- Perform transport calculations with small number of realizations (e.g. 100)
- Determine statistics of each desired transport response
- If any variances exceed desired value then double number of realizations and repeat the above calculations
- Continue doubling the number of realizations until statistics converge
- Note: simultaneous control of all desired responses (e.g. transmission, reflection, dose, etc.)

Control of spatial discretization error

- For each realization, perform transport calculation on a coarse mesh and a refined mesh
- Estimate spatial error of each desired transport response with Richardson extrapolation:

$$\varepsilon = \frac{f_{fine} - f_{coarse}}{f_{fine}} \qquad E = \frac{\varepsilon}{r^p - 1} \qquad GCI = 3\frac{\varepsilon}{r^p - 1}$$

- If any errors exceed desired value then refine mesh and repeat the above calculations
- Continue mesh refinement until spatial results converge
- Note: simultaneous control of all desired responses (e.g. transmission, reflection, dose, etc.)

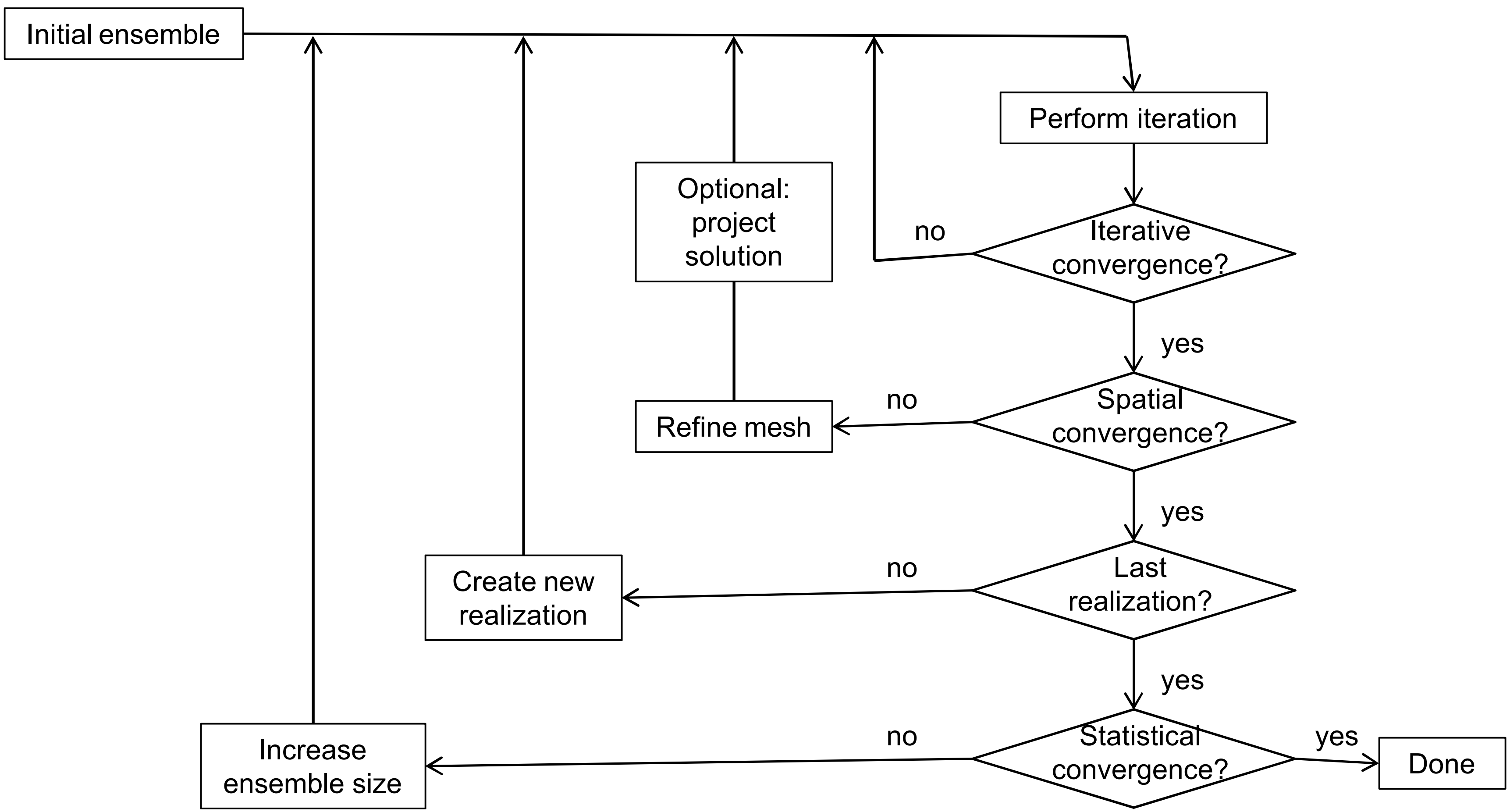
Control of iterative error

- For each realization and level of spatial refinement, perform transport iterations
- Estimate iterative error of each desired transport response as described in companion paper:

$$\left\| r_{rel}^{(l)} \right\| \approx \frac{\left\| x^{(l)} - x^{(l-1)} \right\|}{\left\| x^{(l)} \right\|} \qquad \lambda_{\max,rel}^{(l)} \equiv \frac{\left\| r_{rel}^{(l)} \right\|}{\left\| r_{rel}^{(l-1)} \right\|} \qquad \left\| e_{rel}^{(l)} \right\| \approx \left\| r_{rel}^{(l)} \right\| \frac{\lambda_{\max,rel}^{(l)}}{1 - \lambda_{\max,rel}^{(l)}}$$

- If any errors exceed desired value then repeat the above calculations
- Continue iterations until error estimates converge
- Note: simultaneous control of all desired responses (e.g. transmission, reflection, dose, etc.)

Overall benchmark process



Revisit previous benchmarks

- Benchmark problems taken from Adams et al. (1989).
- Problems consist of nine different Markovian materials and distributions
- Isotropic source on left boundary
- Fixed S_{16} Gauss-Legendre quadrature
- We report only slab widths of 10
- Quantities we examine: reflection, transmission, average flux
- Use Sceptre for transport calculations

Statistical errors

Number of realizations required to obtain 1% error in each quantity of interest

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	1600	12800	100	25600	3200	200	1600	25600	800
$\langle T \rangle$	12800	819200	51200	12800	25600	25600	12800	102400	51200
$\langle \overline{\psi} \rangle$	800	12800	3200	800	6400	3200	800	25600	6400

- Original benchmarks used 10^5 realizations per problem
- Most results overresolved statistically
- Some results not statistically converged

Sandia National Laboratories

Process for examining spatial and/or iterative errors

In order to isolate the spatial and/or iterative errors we examine correlated problems:

- Generate 100 realizations for a given problem
- Compute highly resolved results for these realizations
- Separately compute results using proposed error control mechanisms
- Compare corresponding results for each realization
    - Fraction of realizations with excessive error
    - Error in ensemble average

Sandia National Laboratories

Fraction of realizations exceeding desired (10^{-4}) spatial error vs. spatial control options

Control variable: $\langle R \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	1	1	1	0.73	1	1	0.92	1	1
$\langle T \rangle$	1	1	1	0.73	1	1	0.92	1	1
$\langle \overline{\psi} \rangle$	1	1	1	0.73	0.99	1	0.92	0.69	1

Control variable: $\langle T \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	0	0	0	0.21	0	0	0	0.06	0
$\langle T \rangle$	0.01	0	0	0.28	0	0	0	0	0
$\langle \overline{\psi} \rangle$	0	0	0	0	0	0	0	0	0

Control variable: $\langle \overline{\psi} \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	0.01	0	0	0.40	0.04	0.02	0	0.40	0.05
$\langle T \rangle$	0.68	0.63	0.13	0.60	0.68	0.39	0	0.75	0.29
$\langle \overline{\psi} \rangle$	0	0	0	0	0	0.02	0	0	0

Control variable: $\langle R \rangle \langle T \rangle \langle \overline{\psi} \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	0	0	0	0.01	0	0	0	0.06	0
$\langle T \rangle$	0.01	0	0	0.12	0	0	0	0	0
$\langle \overline{\psi} \rangle$	0	0	0	0	0	0	0	0	0

Ensemble spatial error

Control variable: $\langle R \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	1	1	1	1	1	1	1	1	1
$\langle T \rangle$	0.95	0.4	0.96	0.25	0.6	0.58	0.59	0.16	0.38
$\langle \overline{\psi} \rangle$	0.65	0.26	0.7	0.35	0.54	0.59	0.73	0.18	0.52

Control variable: $\langle T \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	4.3e-5	1.5e-6	1.6e-5	4.0e-4	3.6e-7	1.1e-5	6.0e-5	1.7e-6	3.1e-5
$\langle T \rangle$	2.5e-4	6.1e-5	6.5e-5	2.4e-4	1.1e-6	6.1e-6	1.2e-4	1.5e-5	1.7e-5
$\langle \overline{\psi} \rangle$	2.3e-5	4.4e-6	2.5e-5	1.6e-6	6.4e-7	7.3e-6	1.3e-4	3.4e-6	2.5e-5

Control variable: $\langle \overline{\psi} \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	2.1e-4	2.3e-5	4.6e-5	8.2e-4	1.8e-6	2.6e-4	5.4e-5	7.0e-6	2.7e-4
$\langle T \rangle$	1.0e-3	7.7e-4	2.4e-4	3.9e-4	9.1e-5	2.8e-5	1.1e-4	7.7e-4	1.4e-4
$\langle \overline{\psi} \rangle$	6.5e-5	8.3e-5	8.1e-5	7.5e-6	1.7e-5	6.4e-5	1.1e-4	1.6e-5	1.1e-4

Control variable: $\langle R \rangle \langle T \rangle \langle \overline{\psi} \rangle$

Result	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
$\langle R \rangle$	4.3e-5	1.5e-6	1.4e-5	1.6e-4	3.0e-7	1.1e-5	5.2e-5	9.8e-7	2.6e-5
$\langle T \rangle$	2.5e-4	6.1e-5	5.5e-5	1.2e-4	1.0e-6	6.1e-6	1.1e-4	1.3e-5	1.0e-5
$\langle \overline{\psi} \rangle$	2.3e-5	4.4e-6	2.2e-5	6.8e-6	6.0e-7	7.3e-6	1.1e-4	2.2e-6	1.8e-5

Observations regarding control of spatial errors

- Control based on reflection alone problematic (caused by zero residual after one iteration)
- Results for a particular quantity of interest are generally better when that quantity is controlled
- Best results when all quantities controlled
- Large fraction of realizations with excessive individual errors does not generally lead to grossly excessive error in ensemble average

Fraction of realizations exceeding desired (10^{-4}) spatial error vs. iterative control options

Control and measured variable

$\langle R \rangle$

Iterative tolerance	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
1e-4	1	1	1	0.73	1	1	0.92	1	1
1e-5	1	1	1	0.73	1	1	0.92	1	1
1e-6	1	1	1	0.73	1	1	0.92	1	1
1e-7	1	1	1	0.73	1	1	0.92	1	1

$\langle T \rangle$

Iterative tolerance	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
1e-4	0.02	0	0	0.28	0	0	0	0	0
1e-5	0.01	0	0	0.28	0	0	0	0	0
1e-6	0.01	0	0	0.28	0	0	0	0	0
1e-7	0.01	0	0	0.28	0	0	0	0	0

$\langle \overline{\psi} \rangle$

Iterative tolerance	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
1e-4	0	0	0	0	0	0.02	0	0	0
1e-5	0	0	0	0	0	0.02	0	0	0
1e-6	0	0	0	0	0	0.02	0	0	0
1e-7	0	0	0	0	0	0.02	0	0	0

Fraction of realizations exceeding desired (10^{-4}) spatial error vs. iterative control options, fluxes projected with mesh refinement

Control and measured variable

$\langle R \rangle$

Iterative tolerance	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
1e-4	0.01	0	0	0.12	0	0	0	0.06	0
1e-5	0	0	0	0.03	0	0	0	0.06	0
1e-6	0	0	0	0.03	0	0	0	0.06	0
1e-7	0	0	0	0.03	0	0	0	0.06	0

$\langle T \rangle$

Iterative tolerance	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
1e-4	0.74	0	0.11	0.51	0	0.27	0.11	0	0.24
1e-5	0.21	0	0	0.47	0	0.01	0.05	0	0
1e-6	0.01	0	0	0.35	0	0	0.01	0	0
1e-7	0.01	0	0	0.30	0	0	0	0	0

$\langle \overline{\psi} \rangle$

Iterative tolerance	Stochastic distribution								
	1	2	3	4	5	6	7	8	9
1e-4	0.94	0	0.19	0.55	0.05	0.57	0.04	0	0.67
1e-5	0.90	0	0.16	0.54	0.05	0.54	0.04	0	0.66
1e-6	0.89	0	0.17	0.54	0.05	0.54	0.04	0	0.66
1e-7	0.89	0	0.17	0.54	0.05	0.54	0.04	0	0.66

Observations regarding control of iterative errors

- If the starting guess for iterations is zero, then the iterative tolerance need not be very small relative to the desired spatial error
- Projecting the solution on a coarse mesh onto a refined mesh as the starting guess avoids problems with reflection as a control variable
- Projecting the solution interferes with the control of other variables (asymptotic assumption violated), which can only be partly compensated for by using a tighter iterative tolerance

Conclusions

- The simultaneous control of stochastic, spatial, and iterative errors is complicated – it is difficult to control or analyze each separately
- Errors in individual realizations tend to be averaged away in ensemble results
- Need more work
  - Control of reflection variable
  - Projection of fluxes as starting guess
- The above issues may also affect other ensemble-based analyses, not just stochastic benchmarks