SAND2012-6382P

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Examination of Savings Using Weighted Sum Quadrature Calculations in Stochastic Geometries

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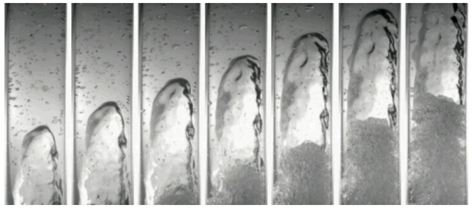
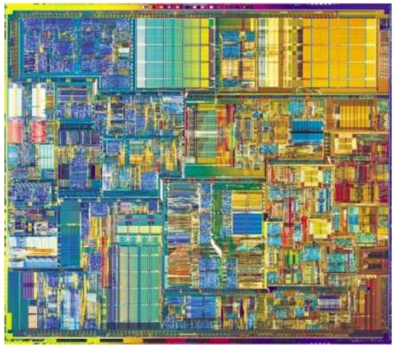
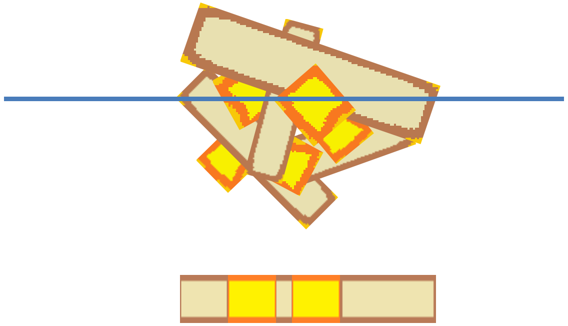
Introduction – Stochastic Media

- Stochastic Media – Two or more materials mixed in a way that cannot easily be exactly modeled
  - Compound mixtures
  - Two-phase flow
  - Small repetitive systems
  - Scalloped Potatoes







Introduction and Outline

• **Old Method – Build Meshes Based on Material Segment Lengths**	• **New Method – Build Meshes Based on Num of Material Segments**

5 slides

– Run many realizations	– With some parameters, run many fewer realizations **(when are there significant savings?)**

2 slides

– Works for all types of mixes	– Works well for mixes with larger segments **(how well?)**

3 slides

– Difficult to integrate with other approaches	– Easier to integrate with other approaches **(such as?)**

1 slide

Both methods run on SCEPTRE (Sandia's Computational Engine for Particle Transport for Radiation Effects)

Two Methods: Poisson Distribution – Two Different Properties

- **Old Method – Material Segment Length**
- **New Method – Number of Material Segments**

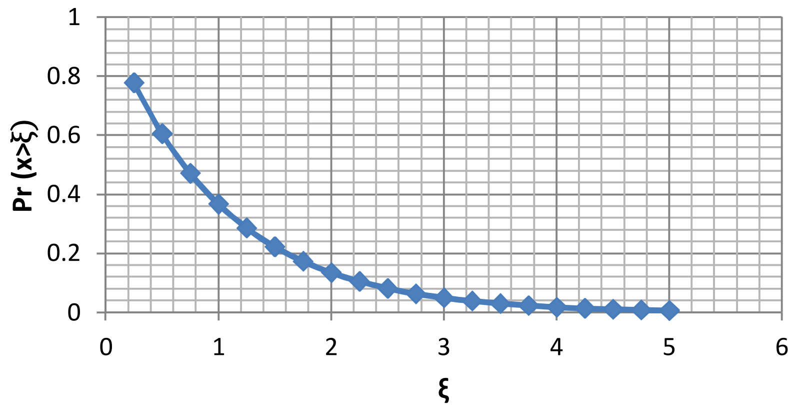
$$\Pr\left(x > \xi\right) = \frac{e^{\frac{-\xi}{\lambda_c}}}{\lambda_c}$$

$$\lambda_c = \frac{\lambda_1 \lambda_2}{\lambda_1 + \lambda_2}$$

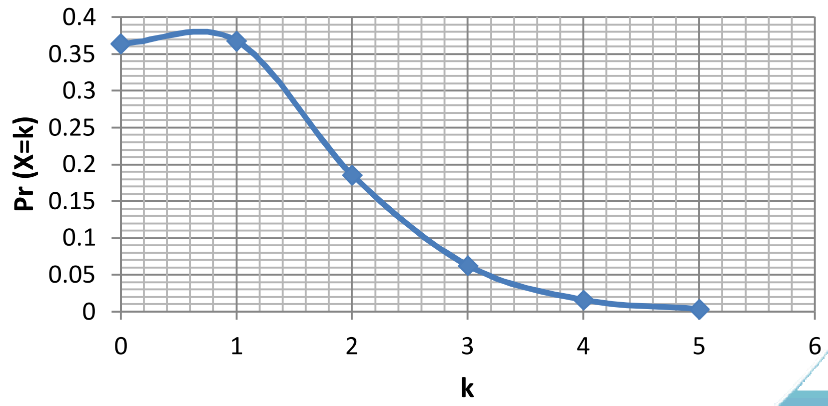
$$\Pr\left(X = k\right) = \frac{\left(\frac{s}{\lambda_c}\right)^k e^{-\left(\frac{s}{\lambda_c}\right)}}{k!},$$

$$for\ k = 0, 1, 2, \ldots$$

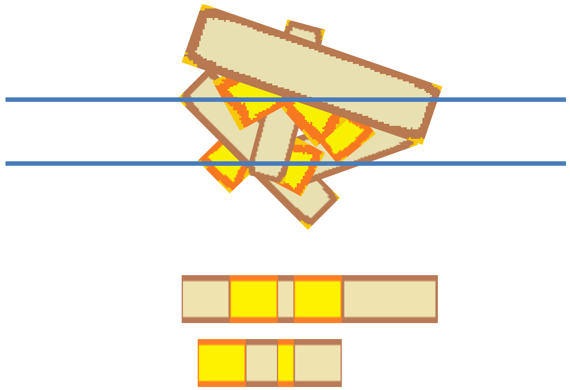
Poisson Distribution – Probability Segment Length > ξ



Poisson Distribution - Probability of Number of Segments



Two Methods: Old Method - Mesh Gen Using Material Lengths



- Meshes built using average material path lengths

- Mesh solved to specified precision: 1 realization

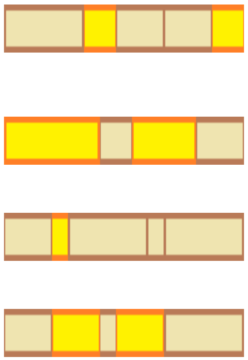
realization 1:

realization 2:

realization 3:

realization 4:

…



- Results from realizations statistically averaged

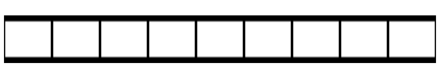
- Oftentimes 10,000 realizations are required for desired precision

Two Methods: New Method – Mesh Gen Using Quadrature & Poisson Weights

- **Sn order (Sn): Number of potential divisions of material segments**
  - Sn = 2

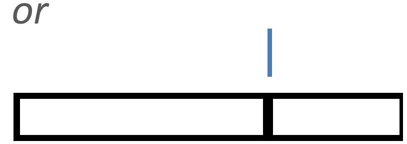
  - Sn = 4

  - Sn = 8



- **Psuedo-interfaces (N): material segment dividers**
  - N = 1, Sn = 2

    - *or*



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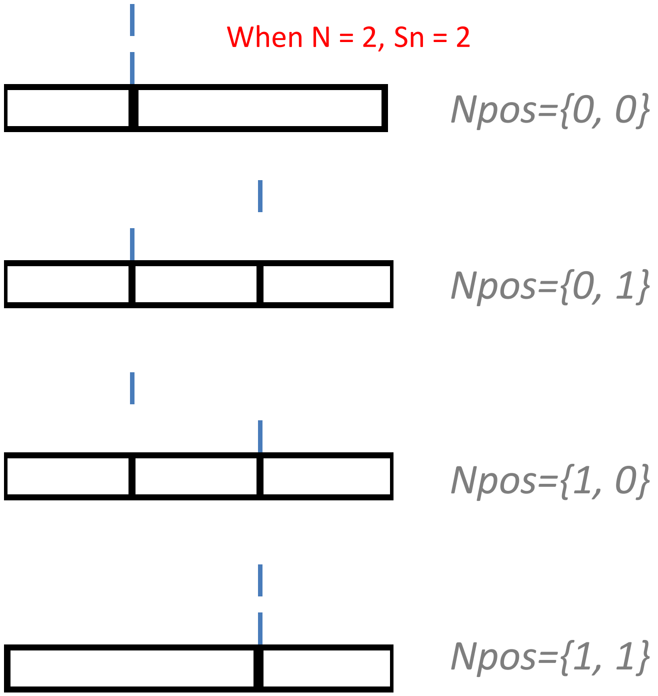
- **Psuedo-interfaces (N): material segment dividers**

Four Geometries

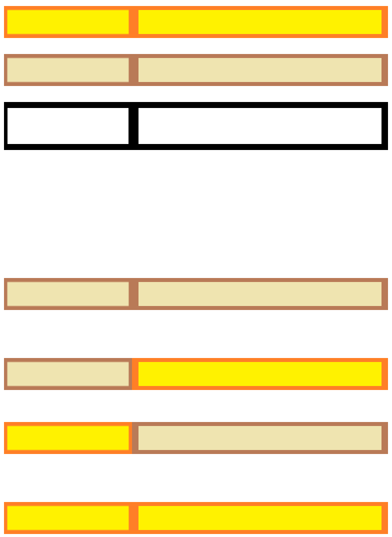
  - N = 2, Sn = 2



Two Methods: New Method – Mesh Gen Using Quadrature & Poisson Weights

- **Each segment must be assigned a material**

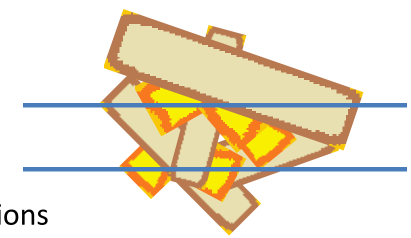
or



so:

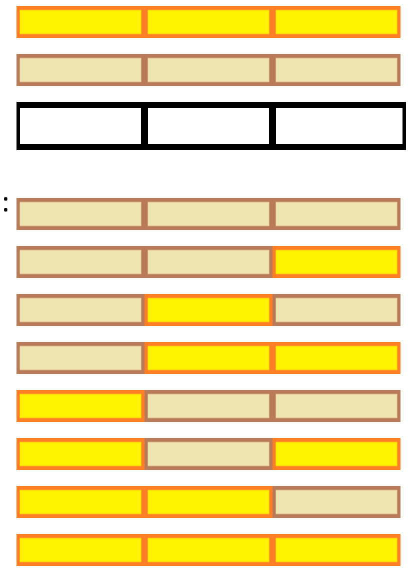
When N = 2, Sn = 2

Geometries: 4
Realizations: 24



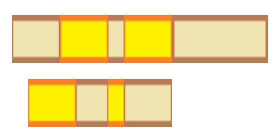
Geom 1: Four meshes: 4 realizations

or



so:

Geom 2: Eight meshes: 8 realizations



Geom 3: 8 realizations

Geom 4: 4 realizations

Total: 24 realizations

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- Easier to integrate with other approaches (such as?)

1 slide

When Are Savings Significant: Quadrature Chart

- **Primary Question: What is it's error?**
  - Need to use greater Sn orders until answer does not change
  - Will need to run large suites of realizations to calculate with large Sn numbers
  - Will need to re-write scripts to accomplish this

Combining Results by Poisson Weights						
			Sn			
		Poisson Wts	2	4	8	16
N	0	0.364182	0.04270 (2)			
	1	0.367861	0.05074 (8)	0.05056 (16)	0.05056 (32)	
	2	0.185788	0.05410 (24)	0.05475 (112)	0.05511 (480)	0.05522 (1984)
	3	0.062555	0.05578 (56)	0.05730 (688)		
	4	0.015797	0.05662 (120)			
	5+	0.003817				
Solution:			0.04887 (210)	(816+)	(512+)	(1984+)

When Are Savings Significant: Remove Redundancies

- **Beast to Tackle – Number of realizations to quantify error**
  - **Program 1: Walks through realization criteria & counts**
  - **Program 2: Enters each geometry and calcs unique material combos**

		Realizations Required to Solve Quadrature Sets				
		Sn Quadrature Order				
		2	**4**	**8**	**16**	**32**
Number of Pseudo-interfaces	**1**	8	16	32	64	128
	2	24	112	480	1984	8064
	3	56	688	6752	59584	500096
	4	120	3760	89184	1733824	
	5	248	18736	1108832		
	6	504	87472	13023840		
	7	364	390448	145185632		
	8	480	1689520			

		Realizations Required: Redundancies Removed				
		Sn Quadrature Order				
		2	**4**	**8**	**16**	**32**
Number of Pseudo-interfaces	**1**	6	10	18	34	66
	2	12	46	186	754	3042
	3	12	102	970	8594	72482
	4	12	132	3070	63194	1151282
	5	12	132	6542	334010	
	6	12	132	10070	1343018	
	7	12	132	12102	4248778	
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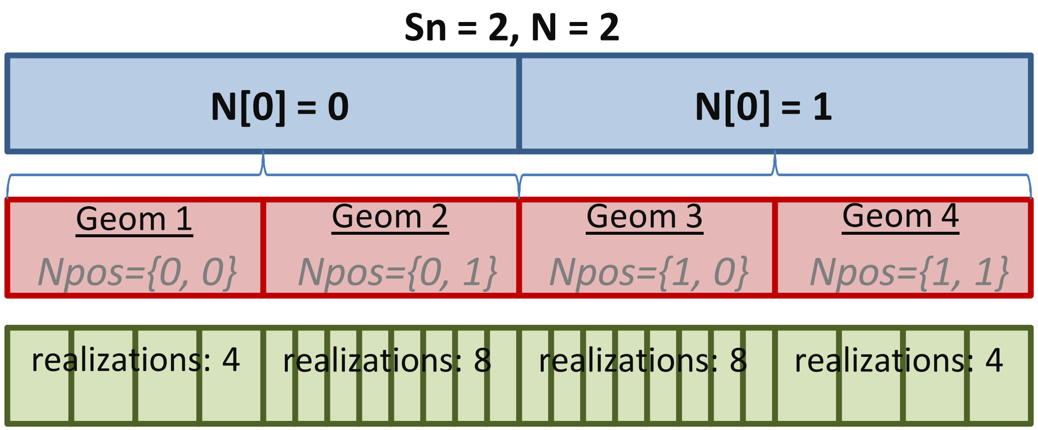
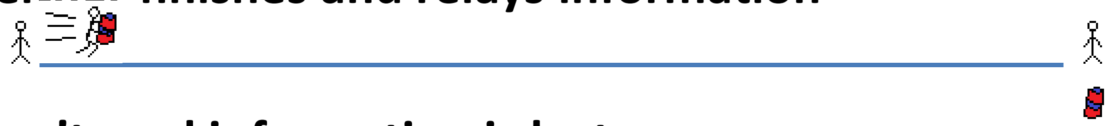
Error Quantification: Original Script

- **Loops of operation**
  - Quadrature placement of first pseudo-interface (12 realizations here)
  - Geometry (4-8 realizations here)
  - Material arrangement (1 realization)



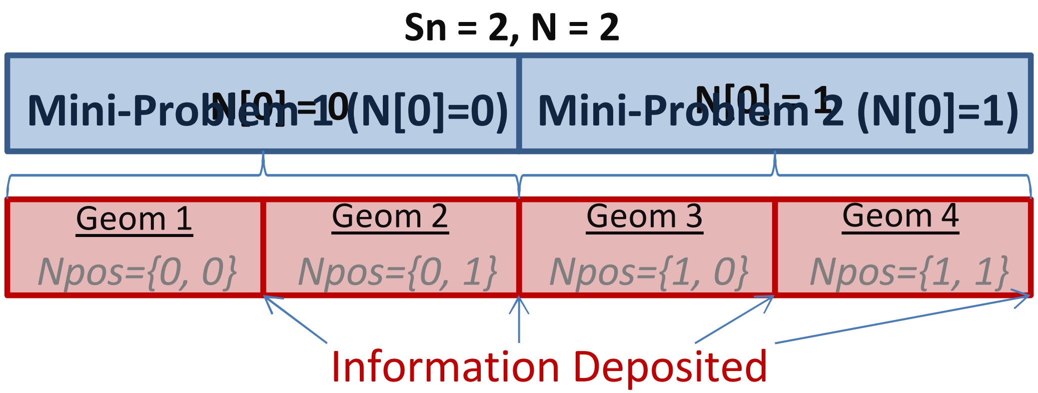
- **Script either finishes and relays information**



- **Or doesn’t, and information is lost**

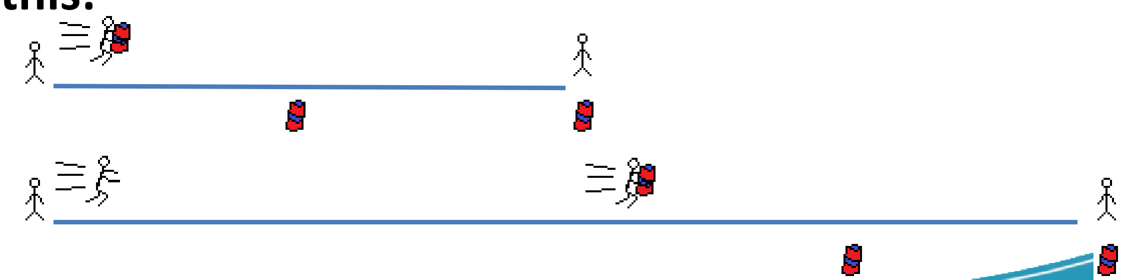
Error Quantification: New Script

- **Features for Calculating Large Realization Sets**
  - **Deposits information at end of every geometry**
  - **Split into mini-problems based on N[0]**
    - *Number of mini-problems possible = Sn order*



- **So this (potentially not finishing and losing all information)**

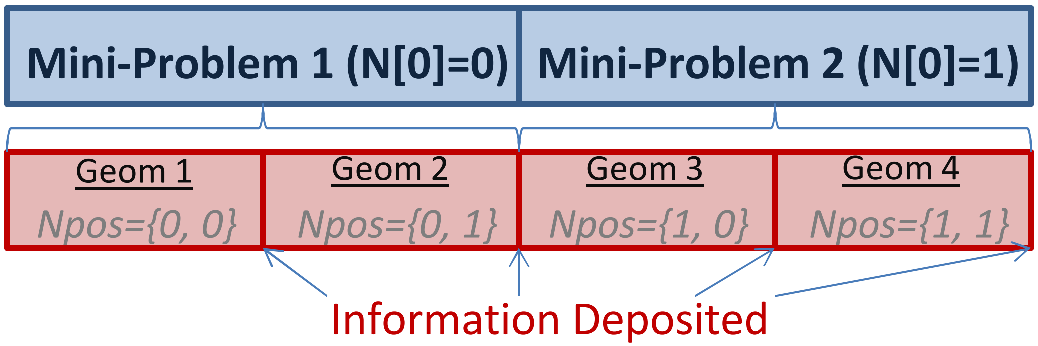
- **Becomes this:**



Error Quantification: Robustness of New Script

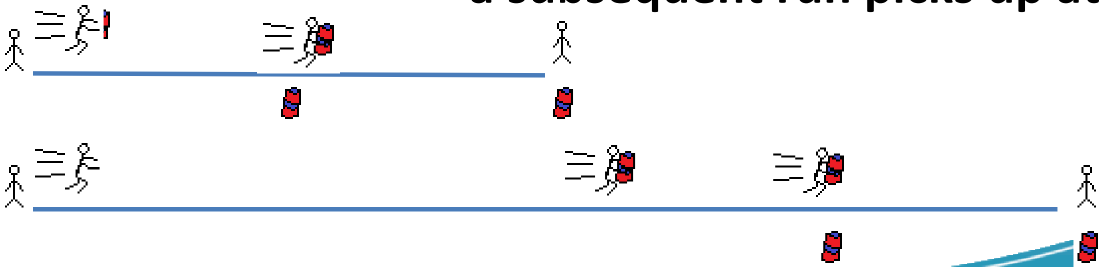
- **Features for Calculating Large Realization Sets**
  - **Deposits information at end of every geometry**
  - **Split into mini-problems based on N[0]**
    - *Number of mini-problems possible = Sn order*

Sn = 2, N = 2



- **So this (potentially not finishing and losing all information)**

- **Let's say a run doesn't finish… a subsequent run picks up at the last deposit**



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Integration With Other Approaches

- **Use Weighted Quadrature Method where efficient, with other approaches where not as efficient (especially larger N values)**
  - **Sparse Grid Quadrature**
  - **Random meshes**

Combining Results by Poisson Weights

		Poisson Wts	Sn 2	Sn 4	Sn 8	Sn 16
	0	0.364182	0.04270 (2)			
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N	2	0.185788	0.05410 (24)	0.05475 (112)	0.05511 (480)	0.05522 (1984)
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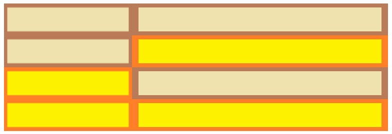
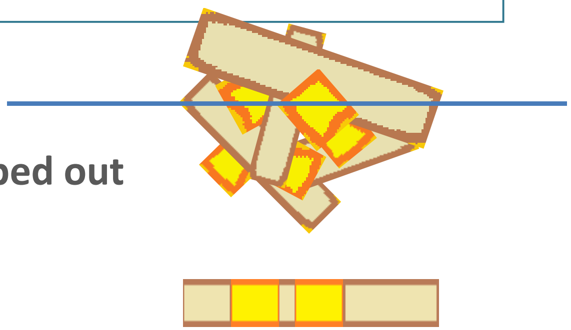
Solution:			0.04887 (210)	(816+)	(512+)	(1984+)

Conclusions/Future Work

- **Conclusions**
  - New Method good in low Sn, low N problems – how well mapped out

realization 1:





  - Can improve more by removing redundancies – will get to later

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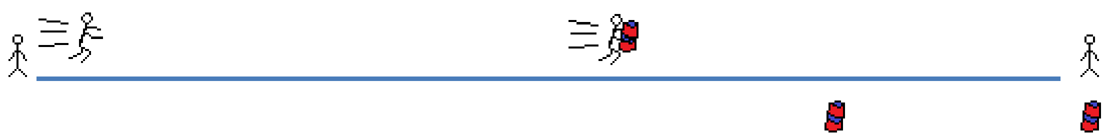
- **Future Work**
  - Will quantify present error in representative cases using newly developed scripting tools – rest of summer



  - Look into integration of other methods – hopefully get to touch this summer

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Acknowledgements/References

Thanks To:

Mentor – Shawn Pautz

Collaborators – Brian Franke, Anil Prinja

Technical and Coding Help – Clif Drumm, Mike Rigley, Ayesha Athar, Google

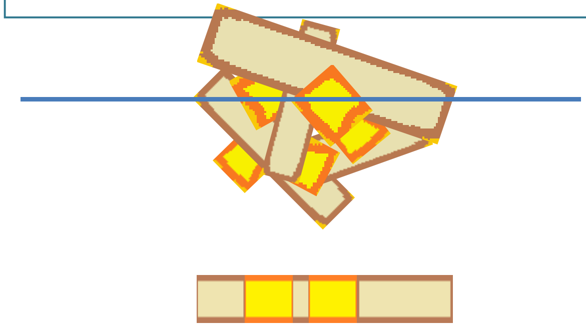
SERRI and Everything Else – Trish St. John

References:

-M. L. Adams, E. W. Larsen, G. C. Pomraning, "Benchmark Results for Particle Transport in a Binary Markov Statistical Medium," *J. Quant. Spectosc. Radiat. Transfer*, 42, pp. 253-266 (1989).

-S. D. Pautz, B. C. Franke, "Generation of Accurate Benchmarks for Transport in Stochastic Media by Means of Dynamic Error Control," *Proc. Int. Conf. on Mathematics and computational Methods Applied to Nuclear Science and Engineering*, Rio de Janeiro, Brazil (2011).

Questions



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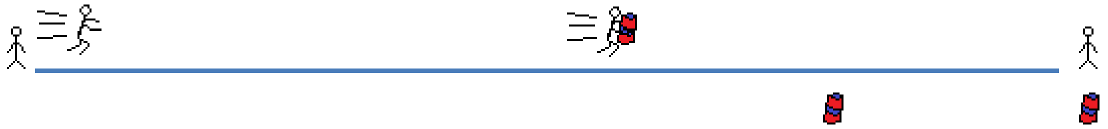
Are There Any Questions?



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