Random Walk Methods and Their Applications to Simulation Problems

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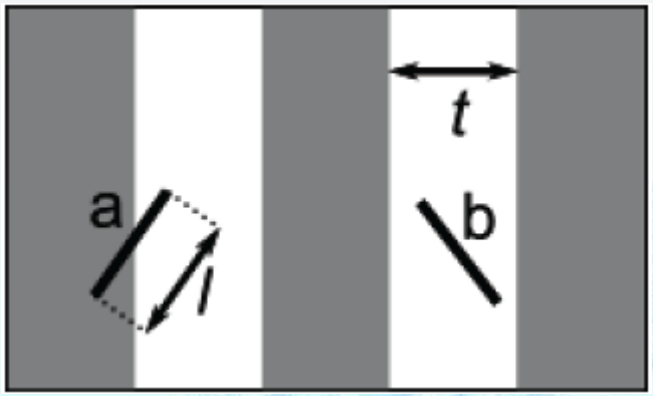
May 30, 2014

Outline

- Monte Carlo Methods
- Random Walk Process and Method
- Discrete Random Walk in Circuit Simulation
- Floating Random Walk in Field Simulation
  - Theory and preliminary
  - FRW for capacitance extraction
  - Biophysical computations
- Conclusions

Monte Carlo Methods

- Early History
  - Probability was first used to understand games of chance
  - Pascal, Fermat, Huygens, Jacob Bernoulli, Laplace (1812: *Théorie Analytique des Probabilités*)
  - Buffon Needle Problem (1777)
    - drop a needle on a lined surface
    - $\pi \approx 2n/m$, where n is the count of experiments, m is count of intersection of needle and grid



Monte Carlo Methods

- Modern Monte Carlo Method
  - Fermi, Ulam, von Neumann, Metropolis, et al., in *Los Alamos National Lab*
  - 1930's, sampling used to estimate quantities in controlled fission / thermonuclear reaction
  - The Name: *Ulam's uncle would borrow money from the family by saying that "I just have to go to Monte Carlo"*
  - After the world war II, digital computer becomes perfect for "statistical sampling"

Monte Carlo Methods

- Classic Examples -- Integration

$$I = \int_0^1 f(x)dx \qquad I \approx \sum_{i=1}^{k} w_i f(x_i)$$

  - Conventional quadrature has the drawback of "the curse of dimensionality" while calculating high-dimensional
  - Estimate with a Monte Carlo process
  - random variable: $x_i \sim U[0, 1]$
  - the score: $f(x_i)$
  - $\bar{I} \sim N(I, \sigma^2)$, σ measures error of $\bar{I}$

Estimate I with the average

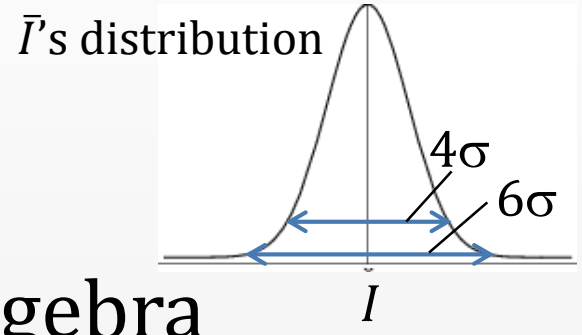
$$I \approx \bar{I} = \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

$$\sigma \equiv \sqrt{var(\bar{I})} = \sqrt{var(f(\xi))/n}, \quad var(f(\xi)) \approx \frac{1}{n-1}\sum_{i=1}^{n}[f(x_i) - \bar{I}]^2$$

error $\propto 1/\sqrt{n}$

Monte Carlo Methods

$$I \approx \bar{I} = \frac{1}{n}\sum_{i=1}^{n} f(x_i) \qquad \bar{I} \sim N(I, \sigma^2)$$



- Classic Examples -- Linear algebra
  - $S = \sum_{i=1}^{m} a_i$, define probabilites $\{p_i\}$ for index i, $\sum p_i = 1$
  - $S = \sum p_i (a_i / p_i)$, i.e., S is the statistical mean of $\frac{a_i}{p_i}$ if a_i is chosen with probability p_i. $S \approx \frac{1}{n}\sum_{i=1}^{n} \frac{a_i}{p_i}$
  - Similar method applies to $S = \sum_{i=1}^{m} a_i x_i$
  - Under certain condition, can even be use to solve a solution component of $\boldsymbol{x} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$, $\rho(\boldsymbol{A}) < 1$

Monte Carlo Methods

- Factors/Features of a Monte Carlo Method
  - Pseudo-random number generator
    - Uniform distribution, nonuniform distribution
  - Parallelization
    - Many independent works due to sampleing nature
    - Synchronization is only needed for computing overall mean and variance (checked infrequently)
  - Minimal memory usage
    - No geometry discretization
    - Memoryless Markov process (no intermediate data)
  - Runtime
    - Convergence rate; computation for each sampling

Monte Carlo Methods

- Morden Applications of Monte Carlo Method
  - Methods for partial differential and integral equations based on random walks (Markov process)
  - Random walk based method for linear algebra
  - Generation of random fields
  - Stochastic ODEs and PDEs
  - Uncertainty quantification (UQ)
  - Financial computing
  - … …

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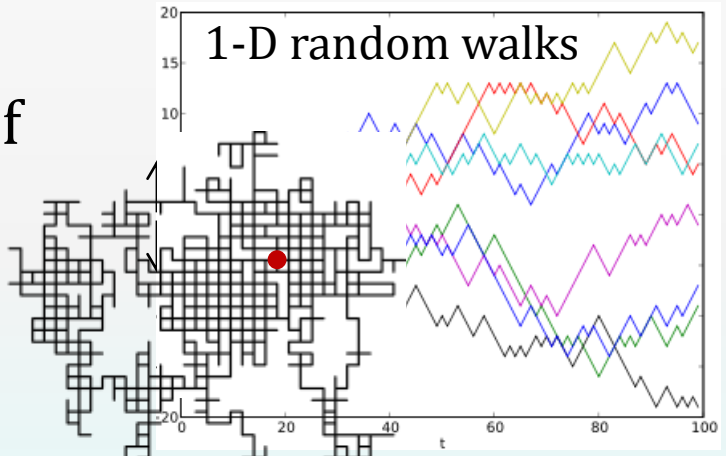
Random Walk Process and Method

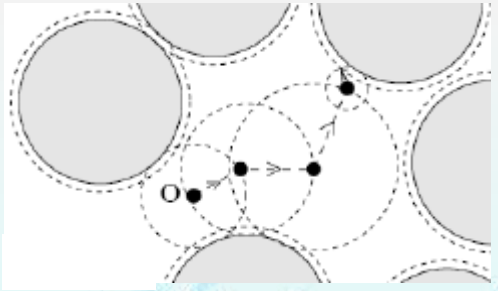
- Definition
  - *A mathematical formalization of a path that consists of a succession of random steps*
  - Abstraction of the phenomenon of particle's Brownian motion
  - *A fundamental model for the recorded stochastic activity*
  - Markov process: can predict the future of the process based solely on its present state (memoryless)
  - Countable state space (*Markov chain*)



A random walk on 2-D lattice

Random Walk Process and Method

- Classification of Random Walk Methods
  - A category of the general MC methods for numerical computation
  - Solve system of linear equations
    - Discrete random walk (*DRW*) on a predefined grid
  - Solve PDE (potential field)
    - Walk on sphere (*WOS*), floating random walk (*FRW*)
    - Other technique (WOB, etc) with limited applications



Markov process on a continuous state space

Random Walk Process and Method

- Pros
  - Locality: calculating local solution, instead of the global solutions
  - Stability: only statistical error; gradually decreases
  - Low memory cost: geometric meshless; Markov property; better for large, high-dimentional problems
  - Parallelizable: walks are independent
- Cons
  - Not as general as FDM/FEM/BEM
  - The convergence can be very slow $Err \propto \frac{1}{\sqrt{n}} \Rightarrow Time \propto \frac{1}{Err^2}$

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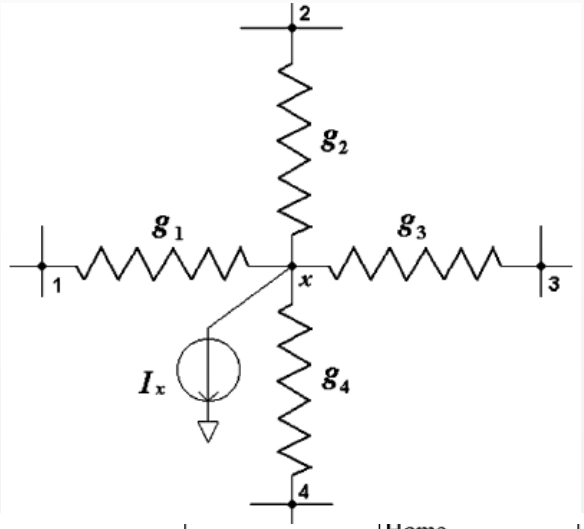
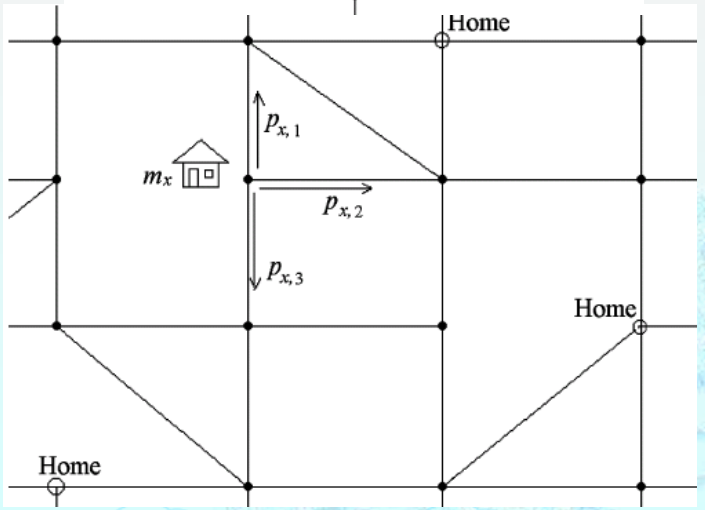
DRW for Circuit Simulation

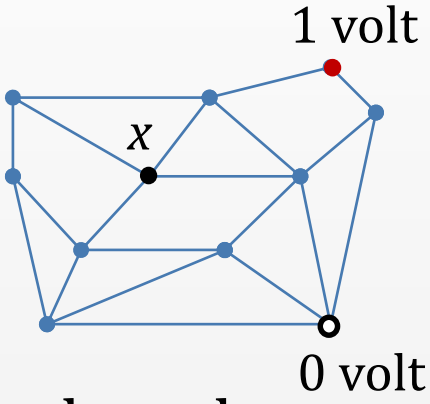
- Circuit Equation
  - $\sum_{i=1}^{degree(x)} g_i(V_i - V_x) = I_x$
  - $V_x = \sum \frac{g_i}{\sum g_i} V_i - \frac{I_x}{\sum g_i}$ cost
  - Regard $p_i = \frac{g_i}{\sum g_i}$ as probability
  - V_x statistically relies to the voltages of neighbor nodes
  - **"random walk game"**
  - *N* random walkers; motel(cost), home(known voltage=reward)
  - V_x = E[total money earned]





DRW for Circuit Simulation

- Probabilistic potential theory
  - 1-volt / 0-volt nodes. node x: $V(x)$= ?
  - A Markov random process: N particles released from x, perform random walks on the grid. Absorption node: 1-volt / 0-volt nodes
  - Probability of a particle reaching 1-volt: $P(x)$= ?
  - Define $p(i \to j | j \epsilon \mathcal{A}_i) = \frac{g_j}{\sum_{j \epsilon \mathcal{A}_i} g_j}$
  - Markov: $P(x) = \sum_{j \epsilon \mathcal{A}_x} p(x \to j) P(j)$



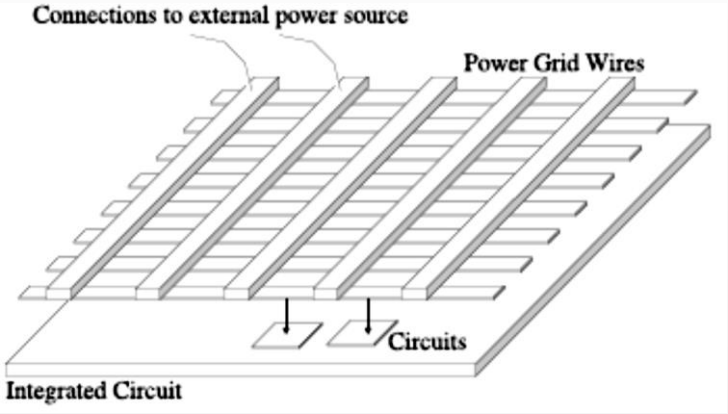
$V(x) = P(x)$

A MC method can be used with RWs

$V(x) \leftrightarrow P(x)$

Generalized if absorption nodes with other voltage

DRW for Circuit Simulation

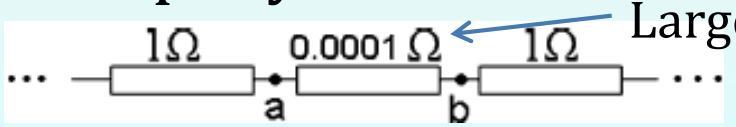


- Application to P/G analysis
  - *Generic random walk*
  - Run a number of random walk path; each includes steps/hops
  - Error $\sim N(0, \sigma^2)$
  - Under fixed confidence level, Time $\propto 1/\text{err}^2$
  - An accuracy-runtime tradeoff
  - Time complexity for each node: $O(N_{walk}N_{hop})$
  - number of walks, average length of a walk

99.7% for err=3σ

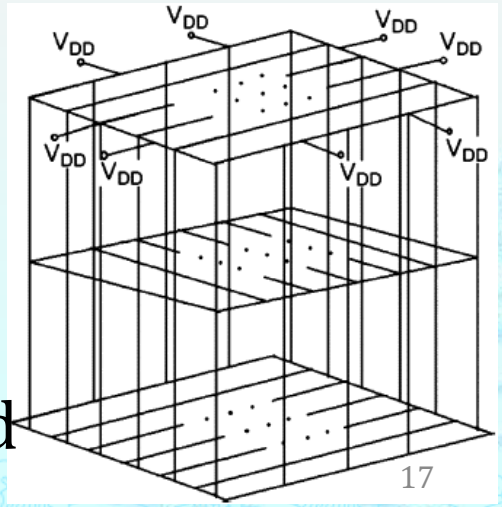
DRW for Circuit Simulation

- Tricks to speed up
  - Not all nodes need high accuracy; adaptive stopping criterion for different node voltage
  - Once a high-accuracy result of a node is obtained, it can be set as a new "home"
  - Truncate very long walk path (limiting L=#step)
- Factors limiting the efficiency
  - "Trap" by isolated low resistance



Larger g_i, p_i

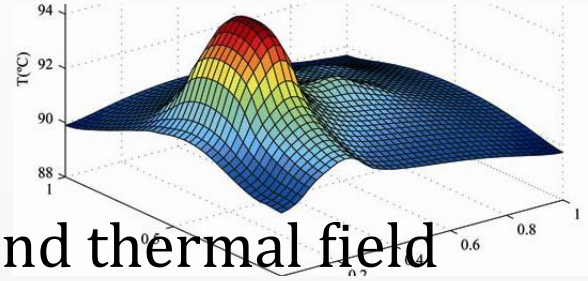
  - Smaller resistances of lower-layer power wires; barrier for walk upward



DRW for Circuit Simulation

- Further techniques for P/G analysis
  - Feasible for transient simulation (*"travel back time"*)
  - Walks reused for different time points (*"bookkeeping"*)
  - Hierarchical RW with macromodeling local grids is *several* to *more than ten* times faster [TCAD'2005]
  - Importance sampling [GLSVLSI'2011]; Backward random walk for incremental analysis [TODAES'2014]
  - Advantages over traditional P/G solver methods
    - Easy speed-accuracy tradeoff
    - Solving a small number of nodes
    - Easy for parallel computing

DRW for Circuit Simulation



- Problem of thermal analysis
  - Equivalence between electrical field and thermal field

	steady electric current field	thermal field	electrostatic field
Equation:	$\nabla \cdot (-\sigma \nabla \phi) = \tau$	$\nabla \cdot (-k \nabla T) = p$	$\nabla \cdot (-\varepsilon \nabla \phi) = \rho$
Quantities	potential ϕ	temperature T	potential ϕ
	conductivity σ	conductivity k	permititity ε
	source density τ	power density p	charge densityρ
	current density D	heat flow density Q	displacement D
	current I	power P	charge Q

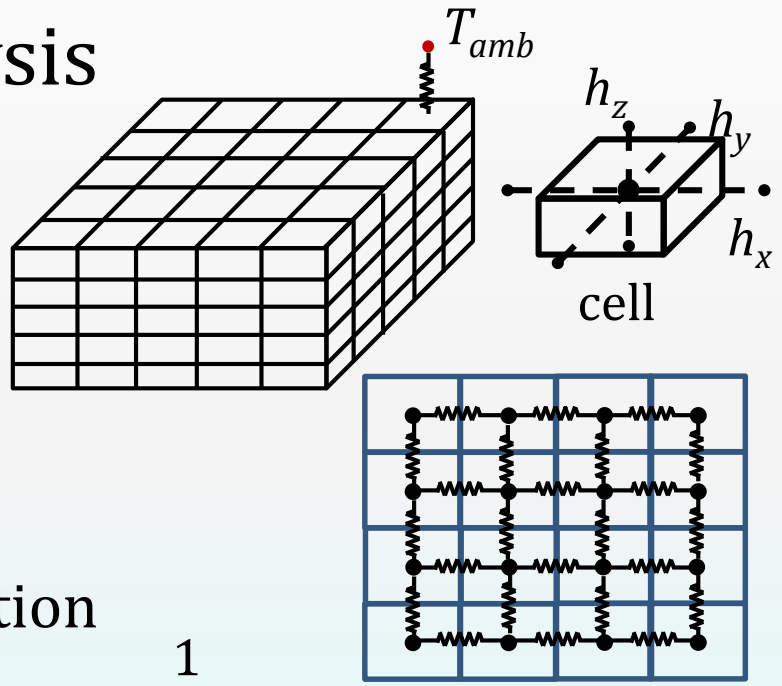
  - Finite volume discretization obtain "*thermal circuit*"

DRW for Circuit Simulation

- Problem of thermal analysis
  - Finite volume method
  - Circuit with thermal resistors
  - Like P/G grid, can be solved with DRW
  - Difficulty
    - Convective boundary condition

$$\kappa \frac{\partial T}{\partial n} + h(T - T_{amb}) = 0, \qquad R_{amb} = \frac{1}{h \cdot h_x h_y}$$

    - R_{amb} is much larger, make it hard to reach "home"
    - Much larger number of nodes



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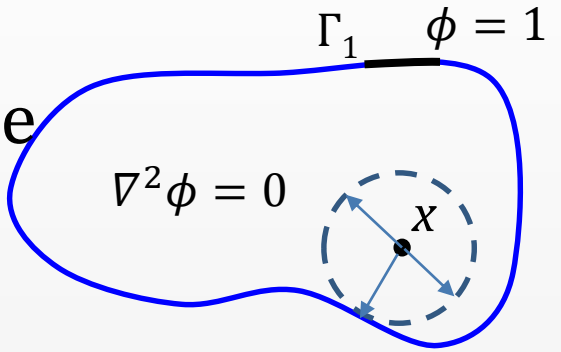
FRW for Field Simulation

- MC method for linear elliptic and parabolic problems
  - Electrostatic: $\nabla \cdot (-\varepsilon \nabla \phi) = \rho$
  - Diffusion of point-like particles: $\nabla \cdot \nabla \rho = 0$
  - Thermal problem: steady state $\nabla \cdot (-k \nabla T) = p$
  - transient state $\nabla \cdot (k \nabla T) + p = \frac{\partial T}{\partial t}$
  - Laplace equation, Poisson equation, parabolic equation
  - Other general equations
- With finite difference (volume) discretization, DRW applies. *It's better to directly solve with FRW*

Probabilistic Potential Theory

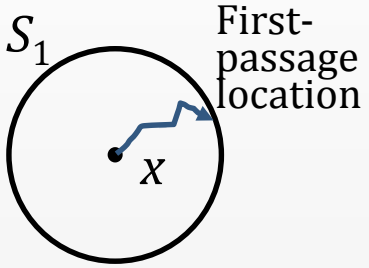


- A simple Dirichlet problem of Laplace
  - Calculate the potential at point x
  - We define a *spherical random process*: the particle always hops from center to sphere surface; terminates (absorbed) at boundary
  - The probability of particle reaching Γ_1 boundary P(x)=?
  - There is a correspondence between P(x) and $\phi(x)$
  - For each hop, if have $\phi(x_k) = \oint_S P_r(x_{k+1}, x_k)\phi(x_{k+1})\mathrm{d}s$
  - $P_r(x_{k+1}, x_k)$ is the PDF for one-step transition in Markov
  - The equations for P(x) and $\phi(x)$ are just the same !
  - MC with initiating particles from x can calculate $\phi(x)$

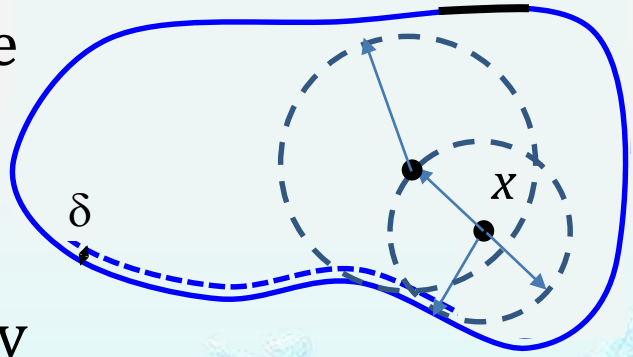
Walk on Sphere Method

- Walk on sphere (WOS) method
  - Integral for potential

$$\phi(x) = \oint_{S_1} P_1(x, x_1)\phi(x_1)\mathrm{d}s$$

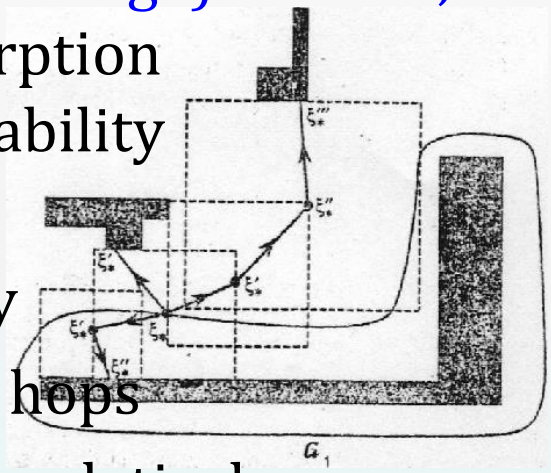


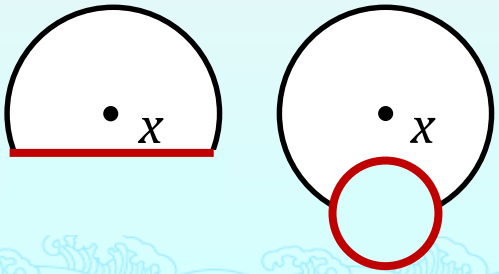
  - For homogeneous material, $P_1 \sim$ uniform distribution
  - Spherical random process is feasible
- Drawbacks
  - Touching threshold δ causes error
  - Small hop near absorption boundary
  - Not good for inhomogeneous material



Floating Random Walk Method

- Floating random walk
  - Can use general-shape transition (first-passage) domain; Shape depends on the geometry of absorption boundary & the availability of hop probability
  - Green's function first passage (GFFP): includes portions of absorbing boundary
  - Advantage: no threshold δ, reduce small hops
  - Prerequisite: hop probability is a quasi-analytical function or can be tabulated
  - FP domains:





Improve efficiency with memory overhead

Floating Random Walk Method

- Successful applications of FRW
  - Bulk properties (linear functionals of the solution)
  - electrical/thermal conductivity of structural composites
  - permeability of porous media
  - electrostatic free energy of a bio-molecule in solution
  - electrical capacitance between conductors
  - Characteristics of absorption boundary may facilitate highly-efficient GFFP approach
  - *Choice of transition domains (FPs) and their usage in FRW affect efficiency (or efficiency/memory tradeoff)*

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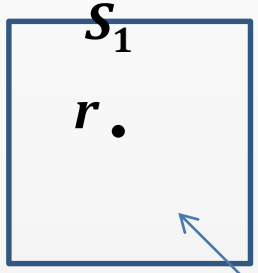
FRW Method for Electric Capacitance

- Integral formula for the potential calculation

$$\phi(\boldsymbol{r}) = \oint_{S_1} P_1(\boldsymbol{r}, \boldsymbol{r}^{(1)}) \phi(\boldsymbol{r}^{(1)}) d\boldsymbol{r}^{(1)}$$



P_1 is called surface Green's function, and can be regarded as a probability density function

- Monte Carlo method: $\phi(\boldsymbol{r}) = \frac{1}{M} \sum_{m=1}^{M} \phi_m$

ϕ_m is the potential of a point on S_1, randomly sampled with P_1

- What if ϕ_m is unknown? expand the integral recursively

$$\phi(\boldsymbol{r}) = \oint_{S_1} P_1(\boldsymbol{r}, \boldsymbol{r}^{(1)}) \oint_{S_2} P_1(\boldsymbol{r}^{(1)}, \boldsymbol{r}^{(2)}) \cdots$$

$$\oint_{S_k} P_1(\boldsymbol{r}^{(k-1)}, \boldsymbol{r}^{(k)}) \phi(\boldsymbol{r}^{(k)}) d\boldsymbol{r}^{(k)} \cdots d\boldsymbol{r}^{(2)} d\boldsymbol{r}^{(1)}$$

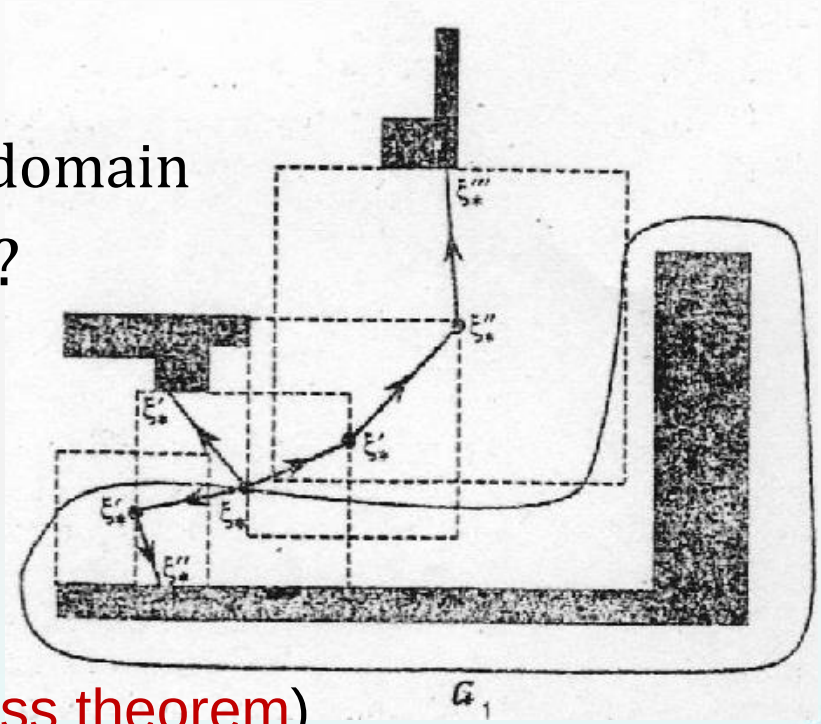
This spatial sampling procedure is called **floating random walk**

FRW Method for Electric Capacitance

- A 2D example with 3 walks
  - Use maximal cube transition domain
- How to calculate capacitances?

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \end{bmatrix}$$

$$\Rightarrow \boldsymbol{Q_1 = C_{11} V_1 + C_{12} V_2 + C_{13} V_3}$$



Integral for calculating charge (Gauss theorem)

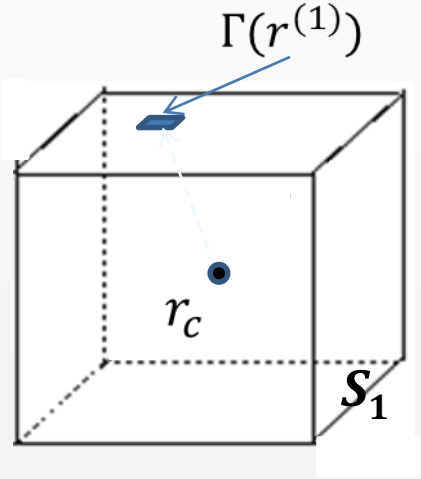
$$Q_1 = \oint_{G_1} F(\boldsymbol{r}) \cdot \hat{n} \cdot \nabla \phi(\boldsymbol{r}) d\boldsymbol{r} = \oint_{G_1} F(\boldsymbol{r}) \cdot \hat{n} \cdot \nabla \oint_{S_1} P_1(\boldsymbol{r}, \boldsymbol{r}^{(1)}) \phi(\boldsymbol{r}^{(1)}) d\boldsymbol{r}^{(1)} d\boldsymbol{r}$$

$$= \oint_{G_1} F(\boldsymbol{r}) g \oint_{S_1} P_1(\boldsymbol{r}, \boldsymbol{r}^{(1)}) \phi(\boldsymbol{r}^{(1)}) \omega(\boldsymbol{r}, \boldsymbol{r}^{(1)}) d\boldsymbol{r}^{(1)} d\boldsymbol{r}$$

weight value, estimate of C_{11}, C_{12}, C_{13} coefficients

FRW Method for Electric Capacitance

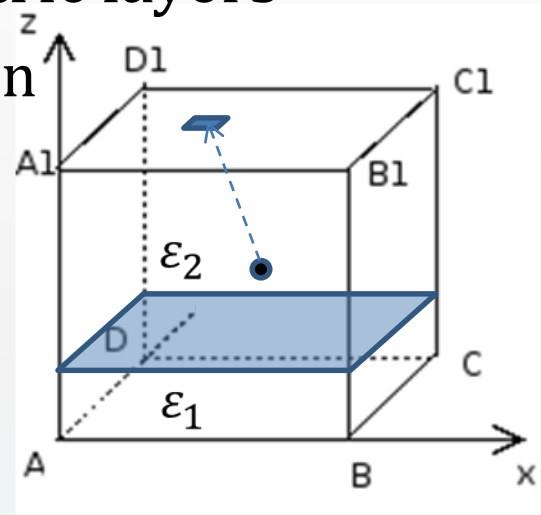
- How to know P_1 for random sampling ?
  - Available for homogeneous transition cube
  - Pre-calculate the probabilities from center to surface panels (GFT)
  - $\omega(\boldsymbol{r}, \boldsymbol{r}^{(1)})$ is also pre-calculated (WVT)

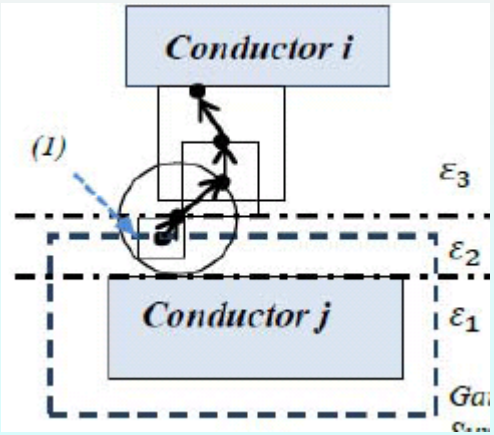


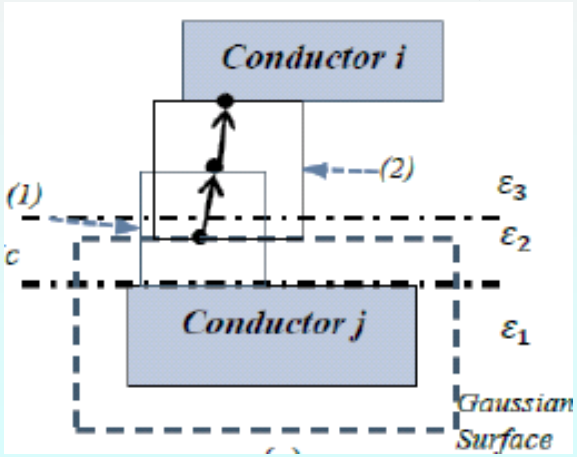
- Efficient FRW for Manhattan geometries
  - Choose cubic transition domain which fits well Manhattan (absorption boundary) interconnects in IC layout
  - Load pre-calculated GFT/WVT for fast sampling on S_k
  - Runtime: $T = N_{walk} N_{hop} T_{hop}$ vs. $T = O(N_{walk} N_{hop})$ for DRW

Treatment for Multi-Dielectric Env.

- IC interconnects are embedded in dielectric layers
  - A recipe is using sphere transition domain
  - Cause frequently stops of a walk
  - For a cube with two dielectric layers, numerically calculate and tabulate GFTs and WVTs (solve a Dirichlet problem)







N_{hop} reduced with some memory overhead

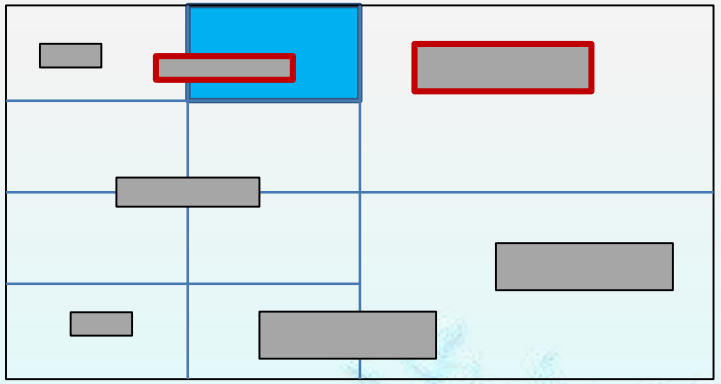
Homogenization and other techniques used in commercial solvers

Space Management for Large Problem

- Problem

$$T = N_{walk} N_{hop} T_{hop}$$

  - T_{hop} (calculate distance to the nearest conductor) increases with the complexity of absorption boundary
  - Space management: decompose whole domain into cells and store local information for faster nearest inquiry
- Basic Octree-based approach
  - *Candidate list* for each node: possible nearest conductors for any point in spatial cell
  - Build by checking *domination*
  - Grow 8 child nodes if the candidate list is so long
  - Largely reduces T_{hop}, with overhead of t_{cons}



Space Management for Large Problem

- The construction of Octree
  - Large case has thousands of conductors, Octree nodes
  - *Simple implementation* causes large t_{cons}: ~ 30 min. for a case with 37062 conductor blocks
  - *The distance limit*: upper bound of the nearest distance to conductor for T
  - Prune domination check with $L(T)$, in Octree construction
  - 600X reduction t_{cons}

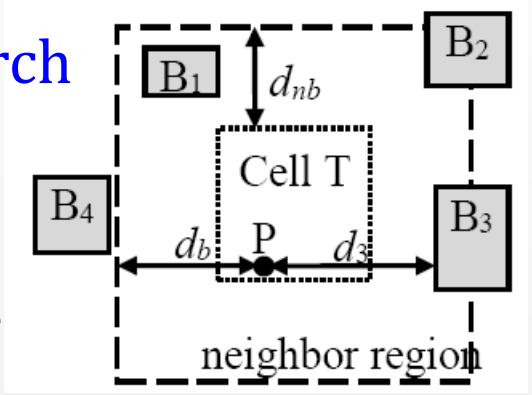
Algorithm 1 CandidateCheck(block B, node T)

1. d := d(B, T); *l* is the size of T;
2. If d ≥ L(T) then return false;
3. For each b in the candidate list of T do
4. If b dominate B then return false;
5. Elseif B dominate b then
6. Remove b from the candidate list of T;
7. Endif
8. Endfor
9. Add B to the candidate list of T;
10. If (d + *l*) < L(T) then L(T) := d + *l*; Endif
11. Return true.

$$L(T)=\min d(B_i, T) + l$$

Space Management for Large Problem

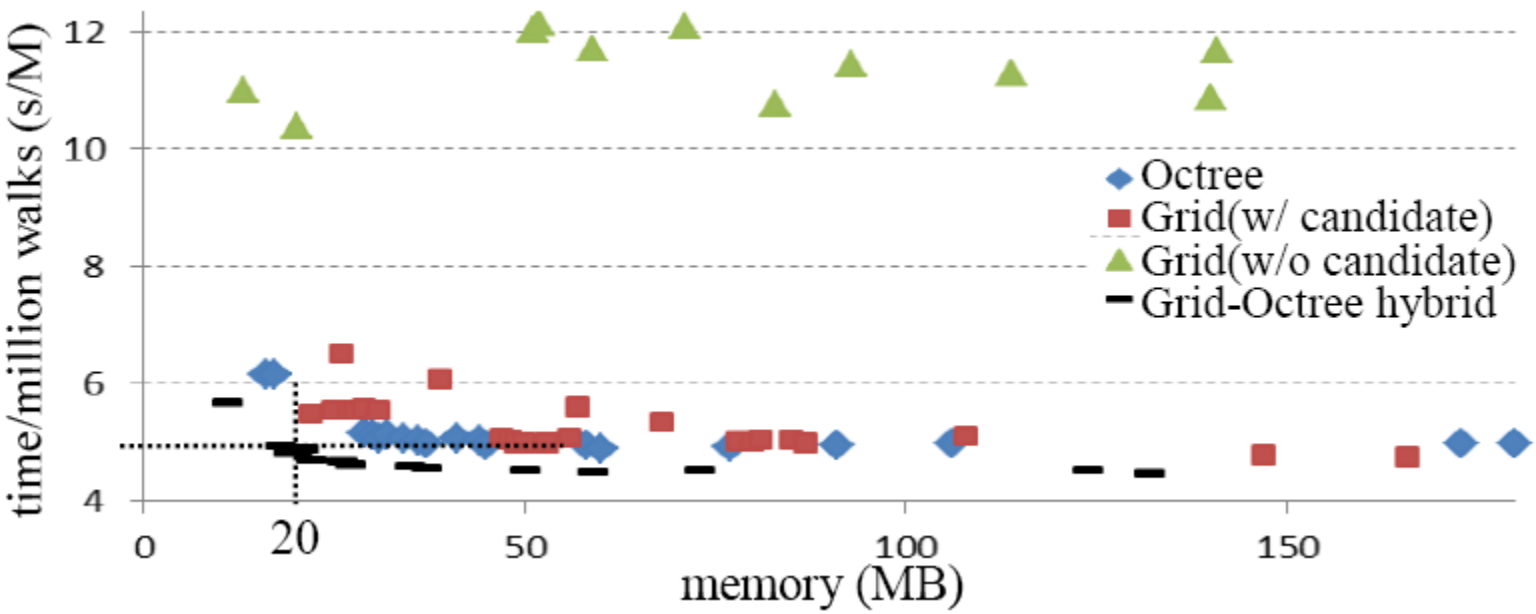
- The construction of the Octree
  - Another idea is the neighbor-region search
  - Reduce t_{cons} by 4~5X again
  - Not guarantee the largest transition cube. But with suitable neighbor setting, this degradation is limited



- A grid/Octree hybrid structure
  - Different spatial structures: K-D tree, Octree, uniform grid, etc.
  - Grid/Octree hybrid: make each node a cube rather than rectangular cuboid when handling large-layout case
  - Code optimization for fast inquiry of the candidate list

Space Management for Large Problem

- Efficiency/memory tradeoff for various spatial strucures



  - Thresholds for node size, candidate list length vary
  - With same memory cost, grid-Octree hybrid structure reduces $N_{hop}T_{hop}$ for >12%
  - With same speed of random walk, it costs half memory

RWCap vs RWCap2 (new space management)

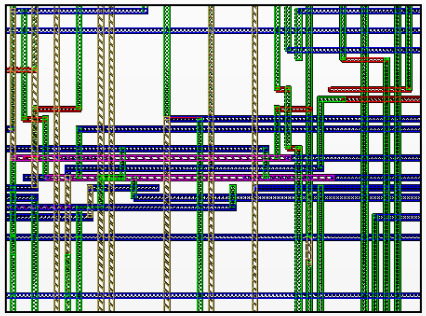
case1: 2000 wire cross-over
case2: "FreeCPU", 37062 blocks
case3: 101595 blocks

case4: 484441 blocks, for which T_{cons} of RWCap2 is only 4.4s

Case	RWCap				RWCap2					Sp. for 1000nets
	T_{cons}	T_{walk} (s)			T_{cons}	Mem	T_{walk} (s)			
	(s)	1 net	100nets	1000nets	(s)	(MB)	1 net	100nets	1000nets	
1	81.3	3.00	304	3185	0.13	6	1.17	119	1178	**2.8**
2	1758	1.80	297	2935	0.34	18	0.80	132	1265	**3.7**
3	16596	1.78	173	1729	1.37	87	0.75	71	718	**25.5**

- Very fast geometric computation makes "best scalability"
- Handle the whole large problem without any approximation
- For cross-over structures, RWCap2 is compared with Rapid3D©
- RWCap2 is 3X faster, while running same #walk

Comparison with Deterministic Methods



- Capacitance extraction for VLSI interconnects
  - Finite difference/finite element method
    - Stable, versatile; slow

    Golden tool: **Raphael**©
  - Boundary element method
    - Fast; not stable (discretization)

    FastCap, **Act3D**©, **QBEM**
  - Floating random walk method
    - Stable (discretization-free); restriction on geometry
    - Scalable/fast, parallelizable

      QuickCap/Rapid3D©, **RWCap**
    - Easy for accuracy-runtime tradeoff

Outline

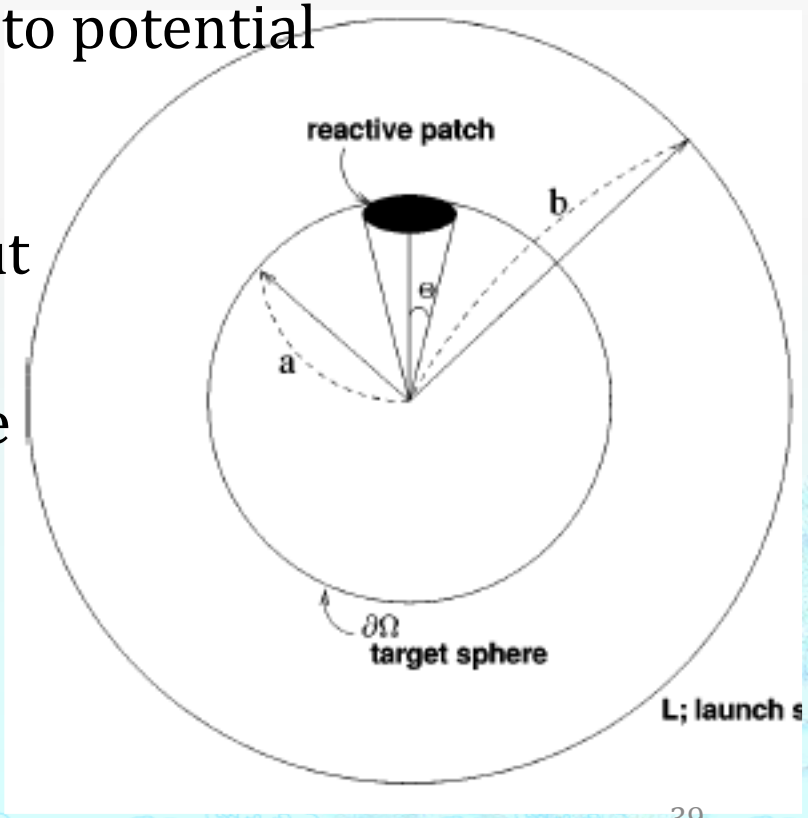
- Monte Carlo Methods
- Random Walk Process and Method
- Discrete Random Walk in Circuit Simulation
- Floating Random Walk in Field Simulation
  - Theory and preliminary
  - FRW for capacitance extraction
  - *Biophysical computations*
- Conclusions

Biophysical Computations

- Diffusion-limited reaction rate
  - A large molecule interacting with small diffusion particles
  - ρ: density of particles, analogy to potential

$$K = \int_{\partial G} D \frac{\partial \rho}{\partial n} ds$$

  - K = capacitance of molecule, but different boundary conditions
  - Walk starts from launch sphere
  - Geometry of the molecule may be complex, union of spheres, with spherical cavity, etc.



Biophysical Computations

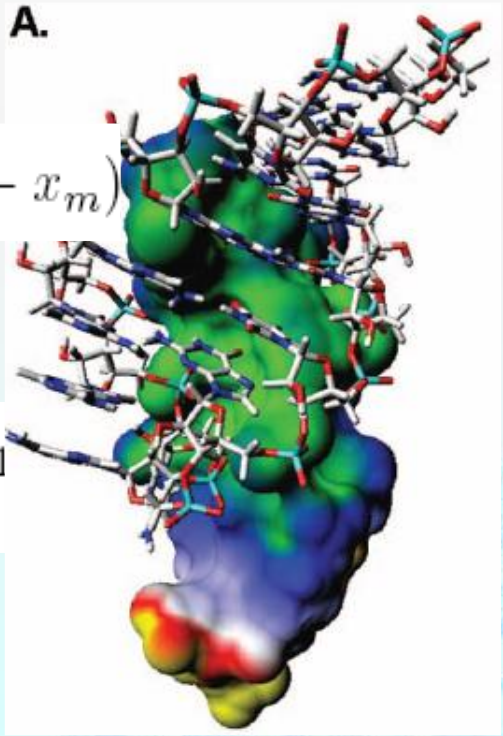
- Internal energy of a molecule
  - Electrostatic effect play a crucial role in structure, stability, dynamics, folding, binding behaviors of biomolecules
  - Every spherical atom has a charge q_m

$$\Delta u(x) = -\frac{1}{\epsilon}\rho(x)\ ,\ x \in G\ ,\ \rho(x) = \sum_{m=1}^{M} q_m \delta(x - x_m)$$

  - In exterior medium, ion distribution follows the Boltzmann law

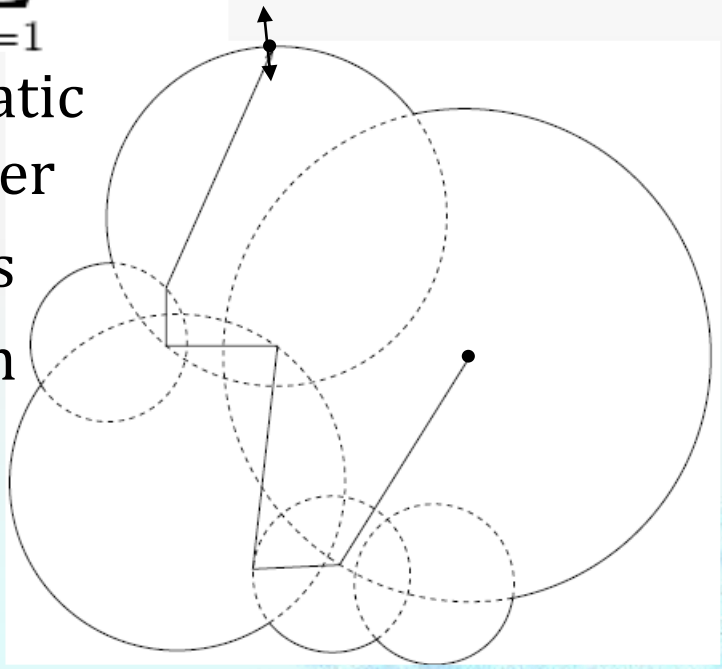
$$\rho(x) = \sum_j q_j^{ion} e n_j \exp(-q_j^{ion} e\ u(x)/k_b T)\ ,\ x \in G_1$$

  - Approximated with linearized Poisson-Boltzmann equation $\Delta u(x) - \kappa^2 u(x) = 0$



Biophysical Computations

- Internal energy of a molecule
  - Electrostatic free energy $E = \frac{1}{2}\sum_{m=1}^{M} u_m q_m,$
  - u_m is nonsingular part of electrostatic potential at the m-th sphere's center
  - G is a union of intersecting spheres
  - Interior medium: Laplace equation
  - A "walk on subdomain" method, avoid distance calculation in WOS
  - Exterior medium: linearized P-B
  - WOS with specific surface Green's function



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Conclusions

- The random walk method is a discretization-free, and reliable computing method
- For calculating a few of local solutions, or linear functionals of solution, RW method is advantageous
- For solving particular PDEs, RW method can outperform the deterministic methods
- Suitable transition domains, pre-calculated transition probabilities, and their usage in the RW procedure are the keys to reduce runtime of FRW

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Thank You !

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