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Monte Carlo method to solve the heat equation in a complex media

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EDstar is a multidisciplinary group that develops Monte Carlo algorithms to model heat transfers.

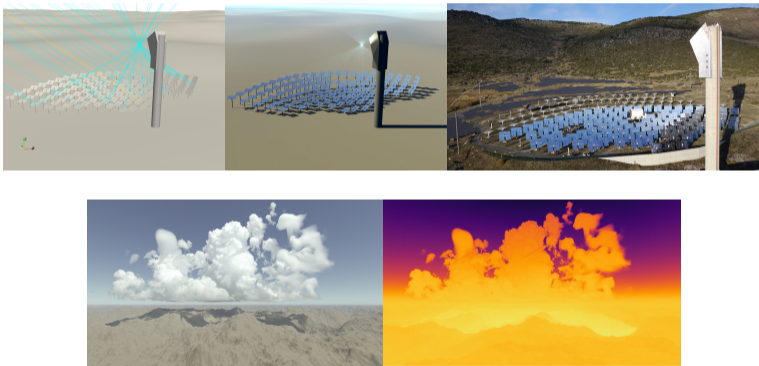


Figure: Images generated by Monte Carlo methods with solstice and htrdr free softwares:

<https://www.meso-star.com/>

An observable expressed as an expectation $\mathbb{E}[w(X)]$ can be estimated by an Integral Formulation Monte Carlo algorithm.

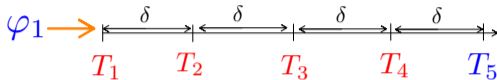
$$\mathbb{E}[w(X)] = \int_{\mathcal{D}} w(x)p_X(x)dx \quad (1)$$

Where:

- $w(X)$ is a weight function that depends on a random variable X
- $p_X(x)$ is the probability density function associated to X

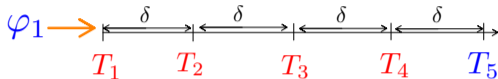
Monte Carlo methods are based on:

- the Law of Large Numbers: $\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N w(x_i) = \mathbb{E}[w(X)]$
- the Central Limit Theorem: the estimate is given with its uncertainty



$$\begin{cases} \Delta T = 0 \\ \varphi_1 \text{ known} \\ T_5 \text{ known} \end{cases} \Leftrightarrow \begin{cases} \frac{d^2 T}{dx^2} = \frac{T(x+\delta) - 2T(x) + T(x-\delta)}{\delta^2} = 0 \\ \varphi_1 = -\lambda \frac{T_2 - T_1}{\delta} \text{ known} \\ T_5 \text{ known} \end{cases} \Leftrightarrow \begin{cases} T_1 = T_2 + \frac{\delta \varphi_1}{\lambda} \\ T_2 = \frac{1}{2} T_1 + \frac{1}{2} T_3 \\ T_3 = \frac{1}{2} T_2 + \frac{1}{2} T_4 \\ T_4 = \frac{1}{2} T_3 + \frac{1}{2} T_5 \end{cases} \quad (2)$$

- The model can be seen as a system of four random variables: T_1, T_2, T_3 and T_4 .
- The expectation $\mathbb{E}(T_1)$ can be evaluated with the mean of weights through a Monte Carlo algorithm (probe computation).



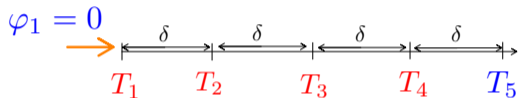
How to evaluate $\mathbb{E}(T_1)$ with a Monte Carlo algorithm?

For each random walk i:

- Starting at point 1, the weight w_i is increased by $\frac{\delta\varphi}{\lambda}$ and the random walker moves to the point 2.
- At points 2, 3 and 4, the random walker flip a coin. If it is "head" the random walker moves to the left, otherwise, it moves to the right.
- Repeat the process while the random walker has not reached point 5 where the weight w_i is increased by T_5 .
- The final weight of the path is: $T_5 + n \times \frac{\delta\varphi}{\lambda}$

$$\begin{cases} T_1 = T_2 + \frac{\delta\varphi}{\lambda} \\ T_2 = \frac{1}{2}T_1 + \frac{1}{2}T_3 \\ T_3 = \frac{1}{2}T_2 + \frac{1}{2}T_4 \\ T_4 = \frac{1}{2}T_3 + \frac{1}{2}T_5 \end{cases} \quad (3)$$

For a large number of random walks, the mean of the weights w_i tends to the expectation $\mathbb{E}(T_1)$.



For the adiabatic case $\varphi_1 = 0 \text{ W/m}^2$

- The final weight of each path is: $n \times 0 + T_5$
- The mean of weight is T_5 and therefore $\mathbb{E}(T_1) = T_5$

- For a 3D geometry, the random walker moves on a sphere of radius δ .
- The algorithm is a meshless method adapted to complex geometries.

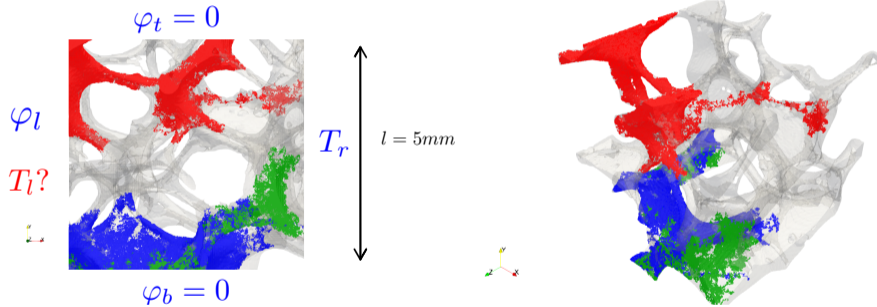


Figure: Three conductive paths sampled with stardis in a porous media to estimate $\mathbb{E}(T_I)$. The geometry is composed of 2.8×10^5 triangles. Sphere radius $\delta = 0.014\text{mm}$. Conductivity of the solid phase is $\lambda = 5\text{W/m.K}$.

The equivalent conductivity along \vec{e}_x is:

$$\bar{\lambda}_x = \frac{l \times \varphi_l}{T_l - T_r} \quad (4)$$

- Monte Carlo: $\bar{\lambda}_x = 4.09 \text{ W/m.K}$
- Finite volume: $\bar{\lambda}_x = 3.99 \text{ W/m.K}$

The absence of mesh becomes more and more interesting when complexity increases!

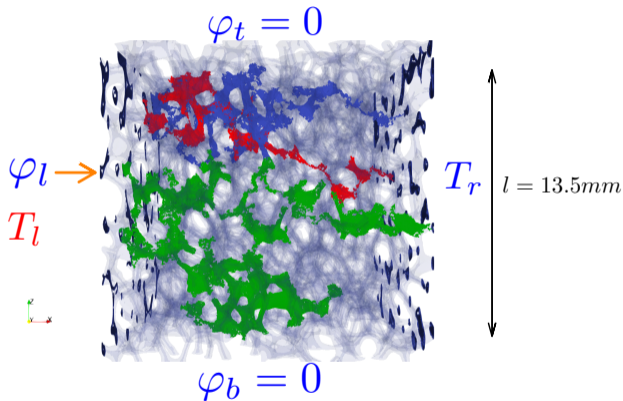


Figure: 3 conductive paths sampled with Stardis in a porous media to estimate $\mathbb{E}(T_l)$. The geometry is composed of 8×10^6 triangles. Sphere radius $\delta = 0.087mm$.

- A Monte Carlo algorithm can easily be parallelised.
- A confidence interval can be computed from the standard deviation.
- The algorithm only evaluate the expectation $\mathbb{E}(T_1)$ or $\mathbb{E}(T_i)$ but not the whole field of temperature (probe computation).
- The coupling between each random variables relies on double randomisation.

Is the method adapted for radiative heat transfers?

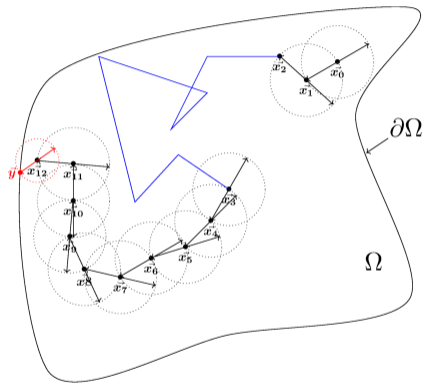


Figure: δ -sphere conductive random walk coupled with a blue radiative path. The path starts at \vec{x}_0 and ends at \vec{y} (Tregan *et al.*, 2023).

Taking radiation into account in transparent or participating media.

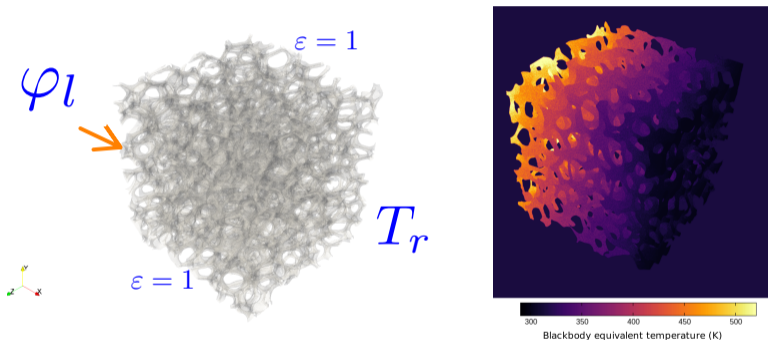


Figure: Infrared rendering of the porous media computed from Stardis software. The fluid medium is transparent and the radiative temperature is 315K. Rendering image resolution is 640 pixels \times 640 pixels. The number of paths per pixel is 500.

Taking into account advection of fluid in pores.

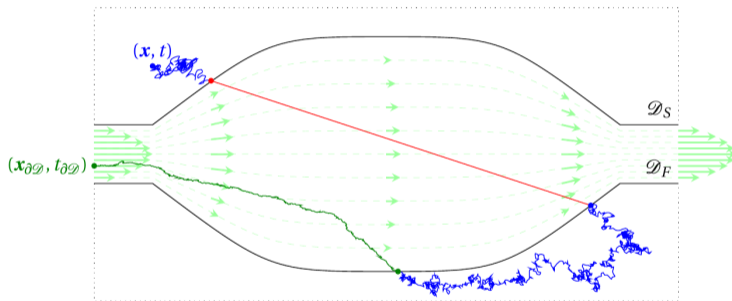


Figure: Advecto-conducto-radiative path in a moving fluid (Ibarrart, 2020). The velocity field is prescribed.

Thanks a lot for your attention. Any questions?

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- Tregan, J. M., et al. 2023. Coupling Radiative, Conductive and Convective Heat-Transfers in a Single Monte Carlo Algorithm: A General Theoretical Framework for Linear Situations. PLOS ONE 18, n° 4
- Villefranque, N., et al. 2022. The “teapot in a city”: A paradigm shift in urban climate modeling. Science Advances 8, n° 27
- Ibarrart, Loris, et al. 2022 Advection, diffusion and linear transport in a single path-sampling Monte-Carlo algorithm: getting insensitive to geometrical refinement.
- Ibarrart, Loris. 2020 Description en espaces de chemins et méthode de Monte Carlo pour les transferts thermiques couplés dans les structures fluides et solides, une approche compatible avec l’informatique graphique. PhD thesis.
- Dunn, W., Shultis, K., 2011. Exploring monte carlo methods. Elsevier.
- Kac, M., 1949. On distributions of certain Wiener functionals. Trans. Amer. Math. Soc. 65, 1–13.
- Feynman, R.P., 1942. The principle of least action in quantum mechanics.

Do you want to try Meso Star free softwares?

- <https://www.meso-star.com/projects/stardis/stardis.html>
- <https://www.meso-star.com/projects/misc/about-fr.html>
- <http://www.edstar.cnrs.fr/prod/fr/>

Express $1 + 4$ as an expected value:

$$1 + 4 = \frac{1}{2} \times 2 + \frac{1}{2} \times 8 = \mathbb{E}[w(X)] \quad (5)$$

"Coin flipping: if I obtain "observe" the outcome of the random variable is 2, otherwise it is 8. I repeat the experiment a large number of time."

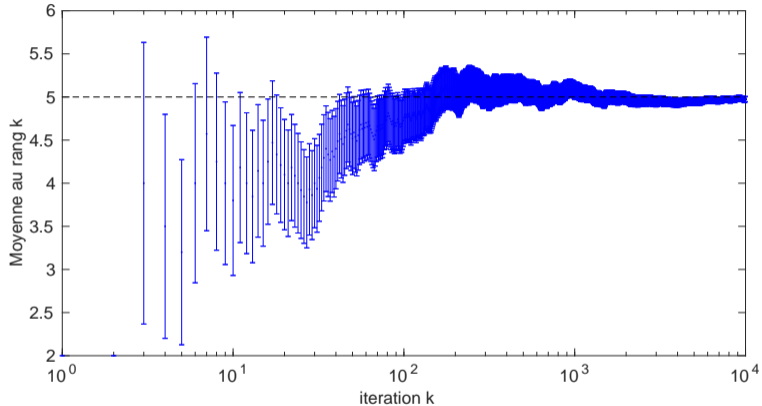


Figure: Convergence to the solution (Confidence intervals at 68 %)

In 1D

$$T(x) = \frac{1}{2}T(x - \delta) + \frac{1}{2}T(x + \delta) \quad (6)$$

In 3D, walk on sphere with a fixed step

$$T(0, \theta, \phi) = \frac{1}{4\pi} \int_{4\pi} T(\delta, \theta, \phi) d\Omega \quad (7)$$

"The average value of T over the surface of a sphere equals the value of T at the center of the sphere" (Dunn, 2011)

Radiative temperature is the temperature that corresponds to radiation balance term ψ_R

$$\psi_R = \psi_{\text{absorbed}} - \psi_{\text{emitted}} = \int_{4\pi} d\vec{u} \int_0^\infty dv k_a^v I_v - \int_{4\pi} d\vec{u} \int_0^\infty dv k_a^v I_v^{\text{eq}} \quad (8)$$

$$\psi_R = 16k_a \sigma T_{\text{ref}}^3 (T_r - T) \quad (9)$$

from Tregan, J. M., et al. 2023. Coupling Radiative, Conductive and Convective Heat-Transfers in a Single Monte Carlo Algorithm: A General Theoretical Framework for Linear Situations. PLOS ONE 18, n° 4

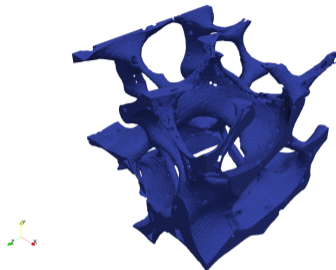


Figure: Porous geometry

$$\overline{\overline{\lambda}}_{MC} = \begin{bmatrix} 4.09 & 0.56 & -0.66 \\ 0.56 & 3.10 & 0.10 \\ -0.66 & 0.10 & 6.96 \end{bmatrix} \quad \overline{\overline{\lambda}}_{\text{finite vol}} = \begin{bmatrix} 3.99 & 1.22 & -1.36 \\ 1.22 & 3.30 & -0.26 \\ -1.36 & -0.26 & 6.73 \end{bmatrix} \quad (10)$$

Assuming that:

- The medium is isotropic and homogeneous
- Thermal properties (c_p , ρ et λ) do not depend on temperature
- Absence of heat source

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \Delta T \quad (11)$$

Reformulation as an expectation:

$$T(\vec{x}, t_{\text{obs}}) = \int_0^\infty \frac{1}{\tau} e^{-\frac{u}{\tau}} du \left\{ \begin{array}{l} T(\vec{x}, t_0) \times H(u - (t_{\text{obs}} - t_0)) \\ \int_{4\pi} \frac{1}{4\pi} d\vec{\omega} T(\vec{x} + \delta\vec{\omega}, t_{\text{obs}} - u) \times H((t_{\text{obs}} - t_0) - u) \end{array} \right. \quad (12)$$