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### GPU-ACCELERATED NUCLEAR MAGNETIC RESONANCE SIMULATIONS THAT RESOLVE A SURFACE ROUGHNESS EFFECT

#### Abstract

Techniques for resolving a surface roughness effect with a GPU-accelerated NMR simulation include identifying, with a graphics processing unit (GPU), a segmented micro-CT image input as a computational domain; assigning, with the GPU, a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating, with the GPU, a random walk numerical simulation with the plurality of random walkers; moving, with the GPU, each random walker of the plurality of random walkers from a previous position to a new position; determining, with the GPU, the new position of each random walker; and updating, with the GPU, an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.

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## Background/Summary

### TECHNICAL FIELD

[0001] The present disclosure describes systems and methods associated with resolving a surface roughness effect on nuclear magnetic resonance (NMR) simulations.

### BACKGROUND

[0002] Pore-scale NMR simulations provide information to laboratory experiments for quantitatively studying complex NMR relaxation behaviors from porous media, including reservoir rocks. The importance of surface roughness on NMR relaxations has been well recognized, as roughness can accelerate NMR decay by providing more pore surface relaxation, which leads to underestimation of pore size distribution. Of particular interest to accurately interpreting the pore size distribution from NMR data include both data from laboratory and field measurements.

Through conventional techniques, it is difficult to resolve the surface roughness effect on NMR simulations due to the non-existence of accurate 3D pore surface roughness measurement methods.

### SUMMARY

[0003] In an example implementation, a computer-implemented method of resolving a surface roughness effect with a GPU-accelerated NMR simulation includes identifying, with a graphics processing unit (GPU), a segmented micro-CT image input as a computational domain; assigning, with the GPU, a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating, with the GPU, a random walk numerical simulation with the plurality of random walkers; moving, with the GPU, each random walker of the plurality of random walkers from a previous position to a new position; determining, with the GPU, the new position of each random walker; and updating, with the GPU, an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.

[0004] In an aspect combinable with the example implementation, determining the new position of each random walker includes determining, with the GPU, that the new position is a pore voxel, with an NMR magnetization of the random walker staying the same with no decline.

[0005] In another aspect combinable any of the previous aspects, determining the new position of each random walker includes determining, with the GPU, that the new position is beyond the computational domain.

[0006] Another aspect combinable any of the previous aspects further includes assigning, with the GPU, the random walker back to a pore voxel or the new position based on a determined boundary condition.

[0007] In another aspect combinable any of the previous aspects, the determined boundary condition is one of a no-flux boundary condition, a periodic boundary condition, or a mirror boundary condition.

[0008] Another aspect combinable any of the previous aspects further includes assigning, with the GPU, the random walker to the new position based on the determined boundary condition and a distance that the random walker travels along an incident angle.

[0009] In another aspect combinable any of the previous aspects, determining the new position of each random walker includes determining, with the GPU, that the new position is a solid voxel.

[0010] Another aspect combinable any of the previous aspects further includes updating, with the GPU, a decline factor to the NMR magnetization of the random walker.

[0011] In another aspect combinable any of the previous aspects, updating the NMR relaxation rate to resolve the surface roughness effect based on the new position of each random walker includes

determining, with the GPU, a surface relaxivity strength for each of the plurality of random walkers based on a spatial heterogeneity of surface relaxivity; and assigning, with the GPU, a relaxation correction factor for each of the plurality of random walkers based on an irregularity of pore geometry.

[0012] Another aspect combinable any of the previous aspects further includes adjusting, with the GPU, the NMR relaxation rate with the relaxation correction factor.

[0013] In another aspect combinable any of the previous aspects, a number of the plurality of random walkers is up to a maximal number of active threads on the GPU based at least in part on a GPU specification and GPU utilization.

[0014] In another example implementation, a graphics processing unit (GPU) includes a plurality of CUDA cores; and at least one memory module configured to store a plurality of instructions that, when executed by the plurality of CUDA cores, causes the plurality of CUDA cores to perform operations. The operations include identifying a segmented micro-CT image input as a computational domain; assigning a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating a random walk numerical simulation with the plurality of random walkers; moving each random walker of the plurality of random walkers from a previous position to a new position; determining the new position of each random walker; and updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.

[0015] In an aspect combinable with the example implementation, the operation of determining the new position of each random walker includes determining that the new position is a pore voxel, with an NMR magnetization of the random walker staying the same with no decline.

[0016] In another aspect combinable any of the previous aspects, the operation of determining the new position of each random walker includes determining that the new position is beyond the computational domain.

[0017] Another aspect combinable any of the previous aspects further includes assigning the random walker back to a pore voxel or the new position based on a determined boundary condition.

[0018] In another aspect combinable any of the previous aspects, the determined boundary condition is one of a no-flux boundary condition, a periodic boundary condition, or a mirror boundary condition.

[0019] Another aspect combinable any of the previous aspects further includes assigning the random walker to the new position based on the determined boundary condition and a distance that the random walker travels along an incident angle.

[0020] In another aspect combinable any of the previous aspects, the operation of determining the new position of each random walker includes determining that the new position is a solid voxel.

[0021] Another aspect combinable any of the previous aspects further includes updating a decline factor to the NMR magnetization of the random walker.

[0022] In another aspect combinable any of the previous aspects, the operation of updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker includes determining a surface relaxivity strength for each of the plurality of random walkers based on a spatial heterogeneity of surface relaxivity; and assigning a relaxation correction factor for each of the plurality of random walkers based on an irregularity of pore geometry.

[0023] In another aspect combinable any of the previous aspects, the operations include adjusting the NMR relaxation rate with the relaxation correction factor.

[0024] In another aspect combinable any of the previous aspects, a number of the plurality of random walkers is up to a maximal number of active threads on the GPU based at least in part on a GPU specification and GPU utilization.

[0025] In another example implementation, an apparatus including a tangible, non-transitory computer-readable memory that stores instructions executable by a graphics processing unit (GPU)

to perform operations. The operations include identifying a segmented micro-CT image input as a computational domain; assigning a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating a random walk numerical simulation with the plurality of random walkers; moving each random walker of the plurality of random walkers from a previous position to a new position; determining the new position of each random walker; and updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.

[0026] In an aspect combinable with the example implementation, the operation of determining the new position of each random walker includes determining that the new position is a pore voxel, with an NMR magnetization of the random walker staying the same with no decline.

[0027] In another aspect combinable any of the previous aspects, the operation of determining the new position of each random walker includes determining that the new position is beyond the computational domain.

[0028] Another aspect combinable any of the previous aspects further includes assigning the random walker back to a pore voxel or the new position based on a determined boundary condition.

[0029] In another aspect combinable any of the previous aspects, the determined boundary condition is one of a no-flux boundary condition, a periodic boundary condition, or a mirror boundary condition.

[0030] Another aspect combinable any of the previous aspects further includes and the operations further include assigning the random walker to the new position based on the determined boundary condition and a distance that the random walker travels along an incident angle.

[0031] In another aspect combinable any of the previous aspects, the operation of determining the new position of each random walker includes determining that the new position is a solid voxel.

[0032] Another aspect combinable any of the previous aspects further includes updating a decline factor to the NMR magnetization of the random walker.

[0033] In another aspect combinable any of the previous aspects, the operation of updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker includes determining a surface relaxivity strength for each of the plurality of random walkers based on a spatial heterogeneity of surface relaxivity; and assigning a relaxation correction factor for each of the plurality of random walkers based on an irregularity of pore geometry.

[0034] In another aspect combinable any of the previous aspects, the operations include adjusting the NMR relaxation rate with the relaxation correction factor.

[0035] In another aspect combinable any of the previous aspects, a number of the plurality of random walkers is up to a maximal number of active threads on the GPU based at least in part on a GPU specification and GPU utilization.

[0036] The details of one or more implementations of the subject matter described in this disclosure are set forth in the accompanying drawings and the description below. Other features, aspects, and advantages of the subject matter will become apparent from the description, the drawings, and the claims.

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## Description

### BRIEF DESCRIPTION OF THE DRAWINGS

[0037] FIG. 1A is a schematic diagram that illustrates a particle distribution at a certain time step of a random walk simulation for a reservoir rock according to the present disclosure.

[0038] FIG. 1B is a schematic diagram of a segmented micro-CT that can be input as a computational domain according to the present disclosure.

[0039] FIG. 2 is a schematic diagram that illustrates a collision of a particle with a solid voxel in a

random walk simulation according to the present disclosure.

[0040] FIG. 3 is a flowchart of an example method for determining a surface roughness effect on nuclear magnetic resonance (NMR) simulations according to the present disclosure.

[0041] FIG. 4 is a schematic diagram of a walker moving from a previous position to a new position in a random walk simulation according to the present disclosure.

[0042] FIG. 5 is a schematic diagram that shows multiple scenarios for the walker moving from the previous position to the new position in terms of different boundary conditions according to the present disclosure.

[0043] FIG. 6 is a schematic diagram that shows a surface roughness effect on NMR T<sub>sub.2</sub> relaxation according to the present disclosure.

[0044] FIG. 7 is a schematic diagram that shows an example workflow of populating a relaxation correction factor to a reservoir rock according to the present disclosure.

[0045] FIGS. 8A and 8B are graphs that illustrate distributions of relaxation inhibition coefficients for two rock samples according to the present disclosure.

[0046] FIGS. 9A and 9B are graphs that illustrate comparisons of NMR T<sub>sub.2</sub> distributions of two rock samples with and without corrections according to the present disclosure.

[0047] FIG. 10 is a schematic diagram that shows a hierarchical structure of threads, blocks, and grids on an algorithmic level for a random walk simulation according to the present disclosure.

[0048] FIGS. 11A-11C are graphs that show GPU performance in executing the NMR numerical simulations according to the present disclosure.

[0049] FIG. 12 is a schematic diagram that shows a comparison of NMR numerical simulations of different examples according to the present disclosure.

[0050] FIGS. 13 and 14 are charts that illustrate comparisons of simulation efficiency and accuracy, respectively, according to the present disclosure.

[0051] FIG. 15 is a table that describes example GPUs according to the present disclosure.

[0052] FIG. 16 shows a schematic drawing of a control system that can be used to perform NMR simulations according to the present disclosure and/or execute any processes described in the present disclosure.

#### DETAILED DESCRIPTION

[0053] The present disclosure describes systems and methods (for example, implemented in microprocessor-based computer hardware and software) for simulating NMR relaxation accelerated by GPU parallel computing to provide critical information to laboratory experiments for investigating complex NMR relaxation behaviors. Example implementations according to the present disclosure include a graphics processing unit (GPU)-accelerated NMR simulator that explicitly accounts for the surface roughness effect in pore-scale NMR simulation. As a numerical simulation, and contrary to laboratory experiments, example implementations according to the present disclosure are controllable and repeatable, which provide additional insights into complicated relaxation mechanisms. Of particular interest to accurate interpretation of the pore size distribution from NMR T<sub>sub.2</sub> responses, the surface roughness effect is advantageously resolved as it accelerates surface relaxation and results into a smaller T<sub>sub.2</sub> relaxation time. Otherwise, data interpreters can underestimate pore size distributions and give incorrect predictions of permeability and fluid types of porous media.

[0054] In some aspects, to effectively control the accelerated surface relaxation, a relaxation correction factor is defined as a ratio of the surface relaxation rate within a spherical pore that honors the same volume with the actual pore geometry to the relaxation rate within the actual pore. In general, the greater the surface roughness effect (or the more irregular the pore shape), the smaller the relaxation correction coefficient. Thus, more corrections are needed to reduce the over-accelerated surface relaxation.

[0055] In some aspects, processes for parameterizing the surface roughness effect on NMR simulations utilize a random walk numerical simulation. In random walk simulations, particles

diffuse in the pore space in the form of Brownian motion, and therefore, the particle movement is quite independent. In addition, collisions between particles are often negligible. These characteristics make a random walk technique particularly suitable for GPU parallel computing according to the present disclosure.

[0056] From the algorithmic aspect, each thread controls a walker and modern GPU hardware can easily have hundreds of thousands threads. For example, implementations according to the present disclosure have been tested on a NVIDIA RTX A6000 GPU. The RTX A6000 GPU has 84 streaming multiprocessors, each of which has 1536 threads at maximum. Theoretically, at 100% GPU utilization, the total number of active threads can reach to 129024. Thus, implementations according to the present disclosure can ideally enable up to 129024 walkers at the same time if running on this GPU (or a similar GPU). The actual performance depends on the GPU hardware and GPU utilization, the latter of which can be affected by the programmed algorithm itself and the finite memory resources on device. Numerical tests show that implementations according to the present disclosure exceed available commercial software in efficiency without compromise in accuracy.

[0057] FIG. 1A is a schematic diagram that illustrates a particle distribution **100** at a certain time step of a random walk simulation for a digital rock sample according to the present disclosure. For example, the particle distribution **100** represents a particular time instant (or step) in a random-walk NMR numerical simulation for a particular reservoir rock (in this example, a Berca sandstone). As shown, spherical balls (one of which is labeled **106**) represent random walkers, which grey shade color indicates a logarithm of magnetization amplitude at base **10** (as shown on scale **102**). Pore space **104** is displayed in a light-grey color to differentiate with the background (solid phase) of the digital rock.

[0058] During a simulation, if a walker/particle collides with a solid voxel, the walker/particle obtains the local surface relaxivity ( $\rho_{\text{sub.i,j,k}}$ ) and relaxation correction factor ( $\alpha_{\text{sub.i,j,k}}$ ) that directly act on the decline factor  $p$ . This is shown graphically in FIG. 2, which shows a schematic diagram **200** that illustrates a collision of a particle **202** with a solid voxel **204** in a random walk simulation according to the present disclosure. By obtaining the local surface relaxivity and relaxation correction factor, this can provide for spatial heterogeneity of surface relaxation with the surface relaxivity at ( $i_{\text{sub.1}}, j_{\text{sub.1}}, k_{\text{sub.1}}$ ) different from surface relaxivities at ( $i_{\text{sub.2}}, j_{\text{sub.2}}, k_{\text{sub.2}}$ ) and ( $i_{\text{sub.3}}, j_{\text{sub.3}}, k_{\text{sub.3}}$ ).

[0059] FIG. 3 is a flowchart of an example method **300** for resolving a surface roughness effect on nuclear magnetic resonance (NMR) simulations according to the present disclosure. Method **300**, in some aspects, can provide a generalized random walk simulation, which, in this example, is used to resolve a surface roughness effect that can accelerate NMR decay by providing more pore surface relaxation, leading to an underestimation of pore size distribution. Thus, by resolving the surface roughness effect can parameterize its impact as an effective coefficient. However, at least some portions of method **300** can also relate to more generalized random walk simulations.

[0060] In some aspects, the method **300** can be executed by an example GPU (such as described in FIG. 15). Method **300** can begin at step **302**, which includes identifying a segmented micro-CT image input as a computational domain. For example, the segmented micro-CT can be input as the computational domain with the solid phase and pore phase represented by 0 and 1 (or vice versa). An example of a segmented micro-CT is shown in FIG. 1B, as image **150**. As shown in the image **150**, a solid phase (background) is in black while the pore phase is made transparent in order to show the inner structure in the image **150**.

[0061] Method **300** can continue at step **304**, which includes assigning random walkers into pore voxels of the segmented micro-CT image. For example, as shown in FIG. 1A, spherical balls **106** represent random walkers, with pore space **104** displayed in a light-grey color to differentiate with the background (solid phase) of the reservoir rock in the segmented micro-CT.

[0062] Method **300** can continue at step **306**, which includes initiating a random walk simulation,

e.g., with a GPU. The random walk simulation can include, for example, up to 129024 walkers at the same time during the random walk simulation.

[0063] Method **300** can continue at step **308**, which includes moving random walkers (for example, each random walker) from a previous position to a new positions This step can occur at each time step of the simulation. For example, FIG. **4** is a schematic diagram **400** of a walker **405** moving from a previous position **407** to a new position **409** in the random walk simulation. As shown in FIG. **4**, positions of the walker **405** can be defined or described through a three-dimensional coordinate system **404** that includes x-axis **406**, y-axis **408**, and z-axis **410**, and its movement is controlled by the angles  $\theta$  and  $\phi$  in a sphere **402** with the radius equal to the diffusing distance,  $ds$  **403**. At each time step of the random walk simulation, all the walkers will be moved to new positions (x.sub.t, y.sub.t, z.sub.t), which center on their previous positions (x.sub.t.sub.0, y.sub.t.sub.0, z.sub.t.sub.0) with the diffusing distance  $ds$  equal to:

[00001]  $ds = \sqrt{6D_0 \Delta t}$ . (1)

[0064] In Eq. (1),  $D_{sub.0}$  is the bulk diffusion coefficient (um.sup.2/s) and  $\Delta t$  is the time step size(s) of the random walk simulation. In some aspects, the diffusing distance is a fraction of the resolution of the digital rock image, which ensures that the random walkers take sufficient steps before encountering a solid surface. The new position **409** of the walker **405** is updated by the following equations:

[00002]  $x_t = x_{t_0} + ds \sin \theta \cos \phi$ . (2)  $y_t = y_{t_0} + ds \sin \theta \sin \phi$  (3)  $z_t = z_{t_0} + ds \cos \theta$  (4)

[0065] In Eqs. (2)-(4), the colatitude angle  $\theta$  and the azimuth angle  $\phi$  range from  $[0, \pi]$  and  $[0, 2\pi]$  respectively. Further, Eqs. (2)-(4) assume the new position **409** (x.sub.t, y.sub.t, z.sub.t) is on the spherical surface (sphere **402**) centering on its position (x.sub.t.sub.0, y.sub.t.sub.0, z.sub.t.sub.0) at the previous time step (position **407**).

[0066] Method **300** can continue at step **310**, which includes a determination of whether the random walker (each random walker) “crosses” a boundary of the computational domain in the movement of the walker in step **308**. For example, there can be three scenarios for walker upon a move to a new position. If the new position is beyond a computation domain (a “yes” determination), then method **300** continues to step **316**, which includes bouncing the random walker back to a pore voxel, the walker is placed back to a pore voxel depending on the boundary condition with no magnetization change. For instance, FIG. **5** is a schematic diagram **500** that shows multiple scenarios for the walker moving from the previous position to the new position when the new position is beyond the computational domain. For example, if a no-flux boundary condition is considered as shown in the diagram **502** (when the walker moves from a “Before” position **501** to an “After” position **503**), then the walker returns along the opposite of the incident direction.

[0067] If the digital rock has a periodic boundary condition, the walker may pass through the boundary to the opposite boundary as shown in the diagram **504** (when the walker moves from a “Before” position **507** to an “After” position **505**) if the new position is inside a pore voxel.

[0068] If a mirror boundary condition is applied, the walker is reflected to a new position, as shown in in the diagram **506** (when the walker moves from a “Before” position **509** to an “After” position **511**). The new position **511**, regardless of the boundary condition, can be calculated such that the total travelling distance is equal to  $ds$ .

[0069] If the new position is in a pore voxel, then the particle (walker) moves to the new position and its magnetization has no decline at this time step. Thus, in this situation, from step **316**, method continues back to step **308**.

[0070] If the determination in step **310** is “no,” then method **300** continues to step **312**, which includes a determination of whether the random walker collides with a solid voxel. If the determination is “yes” in step **312**, then method **300** continues to step **314**, which includes bouncing the walker back to a pore voxel and updating an NMR signal (i.e., NMR magnetization

amplitude) with an adjusting relaxation rate to resolve a surface roughness effect. For example, whenever a walker collides with a solid voxel, it can bounce back to its initial position; or, in a more generic way, it will bounce back to a pore voxel and the new position depends on the inner boundary condition and the distance it travels along the incident angle. Thus, in this situation, from the determination in step **310**, method continues to step **314**. Meanwhile, the NMR signal can be updated by multiplying a decline factor such that:

$$[00003] A_t = A_{t_0} \times (1 - p) \quad (5) \quad \text{with } p = \frac{2}{3D_0} \frac{ds}{dt} \quad (6)$$

[0071] In Eq. 6,  $p$  is the surface relaxivity (in  $\mu\text{m/s}$ ), which is the rock property characterizing the surface relaxation strength,  $ds$  is the diffusing distance (in  $\mu\text{m}$ ),  $D_{\text{sub.0}}$  is the bulk diffusion coefficient ( $\mu\text{m}^2/\text{s}$ ).  $A_{\text{sub.t.sub.0}}$  is the magnetization amplitude at previous time step and  $A_{\text{sub.t}}$  is the magnetization amplitude at the current time step. In conventional random walk simulations, walkers are removed from the simulation based on the finite probability, Eq. (6), to mimic the physical process of nuclear magnetization decay.

[0072] This conventional scheme is adopted by commercial software (for example, PerGeos), while implementations of the present disclosure utilize Eq. 5 (which does not remove walkers). Even though the walker (particle) removal scheme is expected to have less simulation time because the number of particles keep decreasing during simulation, this behavior can reduce GPU utilization. Instead, the number of walkers does not change in the decline factor scheme; threads are created once, and no additional threads become idle during GPU parallel computing. As a result, the high GPU utilization will remain unchanged during the NMR numerical simulation.

[0073] In addition, conventional schemes generally treat surface relaxivity as a particle-carrying parameter. Thus, regardless of which solid voxel a walker hits (collides with moving from an old position to a new position), the walker always has the same surface relaxivity. However, in reality, surface relaxivity exhibits spatial heterogeneity over the rock surface. For this, implementations according to the present disclosure treat surface relaxivity as a solid-carrying parameter and assigns it to solid voxels along the solid-pore interface, as shown in FIG. 2.

[0074] When a walker collides with the solid voxel with the subscript of  $(i, j, k)$ , the local surface relaxivity strength  $p_{\text{sub.i,j,k}}$  controls its NMR amplitude decay. In the same fashion, the relaxation correction factor,  $\alpha_{\text{sub.i,j,k}}$ , is incorporated to control the accelerated surface relaxation due to the surface roughness effect.

[0075] The definition of the relaxation correction factor is detailed as follows. For example, Eq. 6 is multiplied with  $\alpha_{\text{sub.i,j,k}}$  to arrive at:

$$[00004] p = \alpha_{\text{sub.i,j,k}} \left( \frac{2}{3D_0} \frac{ds}{dt} \right), \quad (7) \quad [0076] \text{ to slow the relaxation rate with } \alpha_{\text{sub.i,j,k}} < 1.$$

[0077] Interpretation of pore size distribution from NMR responses often assumes that pore bodies have spherical shapes and smooth surfaces. However, with the surface roughness being overlooked, data interpreters may significantly underestimate pore sizes using conventional analytical solution; since the presence of surface roughness increases the surface area, accelerating the surface relaxation rate shortens the NMR relaxation time.

$$[00005] r = 3 T_{1\text{or}2} \cdot \quad (8)$$

[0078] Eq. 8 associates pore radius,  $r$ , with the  $p$  (the surface relaxivity) and the NMR relaxation  $T_{\text{sub.1}}$  or  $T_{\text{sub.2}}$ .

[0079] Adjusting the NMR relaxation rate to resolve surface roughness effect is graphically shown in FIG. 6. For example, FIG. 6 is a schematic diagram **600** that shows the surface roughness effect on NMR  $T_{\text{sub.2}}$  relaxation. Diagram **600** illustrates NMR  $T_{\text{sub.2}}$  relaxation behaviors in the spherical pore **602** ( $r=10 \mu\text{m}$ ), as well as rough pores **604a-604c** with synthetic roughness. The surface roughness is represented by tetrahedron-shape spikes as shown in the representations of the pores **604a-604c**, which are uniformly distributed on the surface of the pore. The size of synthetic roughness is controlled by a dimensionless parameter,  $\sigma$ . The dimensionless parameter,  $\sigma$ , varies



from 0.1 to 0.3 in pores **604a-604c**, respectively, with the greater value associates with more roughness.

[0080] Note that the created rough pores **604a-604c** honor the same volume as the spherical pore **602**. With  $\sigma$  increasing from 0.1 to 0.3, the NMR T.sub.2 relaxation becomes increasingly faster, showing a sharper magnetization decline in the semi-log graph **620** in FIG. **6**. Graph **620** includes x-axis **622** of time (in ms) and a y-axis **624** of normalized amplitude of NMR T.sub.2 relaxation. Each of the pores **602** and **604a-604c** have associated curves in graph **620** as shown. Graph **650** includes x-axis **652** of NMR T.sub.2 relaxation (in ms) and a y-axis **654** of volume fraction. Each of the pores **602** and **604a-604c** have associated curves in graph **650** as shown. The curves in graph **650** are the so-called NMR T.sub.2 curves. with the x-axis representing the T.sub.2 relaxation time and each value indicates a pore size (see Eq. (8) if the surface relaxivity,  $\rho$ , is known. The y-axis represents the volume fraction of each pore size to the total pore volume. Thus, the NMR T.sub.2 curve is extensively used as an indicator of the pore size distribution.

[0081] Without taking the surface roughness effect into account, the pore radius, calculated from Eq. (8), now is only one third of the actual pore radius (10  $\mu\text{m}$  reducing to 3.5  $\mu\text{m}$ ). Step **318**, therefore, includes resolving a surface roughness effect. The surface roughness effect must be resolved in the NMR simulation that implicitly accelerates surface relaxation. For this purpose, and in step **318**, the relaxation correction factor is defined and incorporated into this invention for effective control of surface relaxation.

[0082] In some aspects, the relaxation correction factor is used to reduce the faster surface relaxation rate in the irregular pore bodies to the normal surface relaxation rate. Thus, it is defined as the ratio of the surface relaxation rate in the equivalent spherical pore that has the same volume with the actual pore bodies to the surface relaxation rate in the actual pore geometry. To calculate the relaxation correction factors for a digital rock, the first step is to divide the connected pore space into disconnected pore bodies. Then, the random walk simulation can be used to calculate the surface relaxation in each disconnected pore geometries. The relaxation rate in the equivalent spherical pore can be calculated by the analytical solution. The relaxation correction factors are then computed based on the above definition and populated back to the digital rock.

[0083] For example, FIG. **7** is a schematic diagram **700** that shows an example workflow of populating a relaxation correction factor to a digital rock according to the present disclosure. The workflow of diagram **700** utilizes a Berea sandstone as an example. In this example, plot **702** illustrates the distribution of the relaxation correction factor in 3D space as an output of the workflow from a digital rock sample **708** (as noted, of Berea sandstone). Disconnected pore bodies **706** from the digital rock sample **708**, as well as equivalent spherical pores of the disconnected pore bodies **706** have NMR decay curves shown in the graphs **704**, which relate NMR relaxation normalized amplitude to time. Curves **703** represent the NMR decay curves of the disconnected pore bodies **706** (the actual curves) while curves **705** represent the equivalent spherical pores of the disconnected pore bodies **706**. As shown in the plot **702**, the darker the color, the smaller the relaxation correction factor. Thus, the actual surface relaxation rate is much larger than the expected surface relaxation rate and more corrections are needed to slow down the surface relaxation.

[0084] Returning to method **300**, subsequent to step **318**, method **300** continues back to step **308**. Further, if the determination in step **312** is “no,” then method **300** continues to step **314**, which include placing the random walker to a pore voxel. Following step **314**, method **300** continues back to step **308**. In some aspects, method **300** can end when a simulation time (for example, a predetermined simulation time duration) has expired. As an example, the simulation shown in FIG. **6** ends upon expiration of a predetermined time duration of 4000 ms or a total magnetization amplitude becomes lower than a threshold value (for example, 10-8).

[0085] Based on the proposed methodology of method **300**, two carbonate samples with the dimension of 512×512×512 were tested. FIGS. **8A** and **8B** are graphs **800** and **850** (respectively)

that illustrate distributions of relaxation correction factors for the two (carbonate) rock samples based on the respective numerical scales **802** and **852**. In this example, the image resolution is  $6.2\ \mu\text{m}$  (in graph **800**) and  $5.5\ \mu\text{m}$  (in graph **850**). To perform the random walk simulation, the number of walkers in this example was set to 100,000, surface relaxivity is  $20\ \mu\text{m/s}$ , bulk diffusion coefficient is  $2500\ \mu\text{m}^2/\text{s}$ , and a no-flux boundary condition is applied.

[0086] FIGS. **9A** and **9B** are graphs **900** and **950** (respectively) that illustrate comparisons of NMR T<sub>sub.2</sub> distributions of the carbonate rock samples in the testing with and without corrections according to the present disclosure. Graph **900** is for a first carbonate rock sample of FIG. **8A**, while graph **950** is for a second carbonate rock sample of FIG. **8B**. In these graphs **900** and **950**, x-axes **902** and **952** represent NMR T<sub>sub.2</sub> relaxation time (in ms), while y-axes **904** and **954** represent volume fraction. Curves **906** and **956** represent the NMR T<sub>sub.2</sub> relaxation with correction for the respective samples of FIGS. **8A** and **8B**, while curves **908** and **958** represent the NMR T<sub>sub.2</sub> relaxation without correction for the respective samples of FIGS. **8A** and **8B**. In graphs **900** and **950**, dotted line curves **910** and **960** represent new T<sub>sub.2</sub> curves for the respective samples of FIGS. **8A** and **8B**.

[0087] As shown in graphs **900** and **950**, the entire distribution shifted to larger T<sub>sub.2</sub> relaxation times without changing the shape of the curve too much. That means, with the help of relaxation correction factors, the surface relaxation rate is effectively controlled and now the NMR T<sub>sub.2</sub> responses could better reflect pore sizes. Even though the relaxation correction factors provide a good manner to control the surface relaxation rate, method **300** is not easy for practical applications since it requires decomposing the connected porous structure into disconnected pore bodies whenever a new digital rock is provided. By analyzing the calculated relaxation correction factors in terms of surface roughness coefficients, it was found that all the data points cluster together, which means a single upscaled coefficient can be sufficient to represent the overall effect.

[0088] In some aspects, a centroid of the point cloud is calculated, giving the upscaled relaxation correction factor equal to 0.66. Instead of using the complex distribution of relaxation correction factors as shown in FIGS. **8A** and **8B**, all the relaxation correction factors can be set to 0.66. The new T<sub>sub.2</sub> curve **910** overlaps with the curve **906** for the first sample. For the second sample, the peak T<sub>sub.2</sub> value (in curve **960**) remains unchanged, but the shape of T<sub>sub.2</sub> curve **960** has some slight change compared to the curve **956**. Overall, the numerical results demonstrate that it is technologically feasible to use one or multiple upscaled coefficients to represent the overall effect a full distribution of relaxation correction factors. This can make the processes described in the present disclosure, with a proposed GPU-accelerated NMR simulator, easier for practical applications.

[0089] As noted, method **300** (and other processes according to the present disclosure) can be implemented with a GPU-accelerated NMR simulator. An advantage of utilizing a GPU-accelerated NMR simulator includes, in some examples, a significant acceleration of a random walk simulation. This can be advantageous to scale up the NMR simulation with high-resolution digital rock models. For example, a high-resolution digital rock may have  $1000 \times 1000 \times 1000$  voxels, with a resolution of 2 to  $3\ \mu\text{m}$ . If the porosity of the rock is 30% and the maximal number of walkers is 10% of the number of pore voxels, there can be 30 million walkers. Such an NMR simulation could be time-consuming and computing-resource consuming, thereby making the example GPU-accelerated NMR simulator desirable.

[0090] FIG. **10** is a schematic diagram **1000** that shows a hierarchical structure of threads, blocks, and grids on an algorithmic level for a random walk simulation according to the present disclosure. To initialize a GPU kernel that is a GPU function called from the host (CPU), the first step is to allocate a sufficient number of threads, each of which controls a random walker. As shown in diagram **1000**, one-dimensional (1D) grids and blocks can be initialized for GPU parallelism. The total number of threads is the product of the grid size and block size. Specifically, the grid size is defined by the blocks per grid, which is a 1D array identifying the number of blocks. Similarly, the

threads per block specifies the number of threads. Diagram **1000** illustrates a kernel function launched with 256 blocks per grid and 256 threads per block. Since each thread controls a walker, the entire grid enables to manage  $256 \times 256 \times 256 = 65,536$  walkers at the same time. With properly programming the algorithm, modern GPU hardware can achieve high utilization with thousands of active threads. Given that each thread controls a walker doing the random walk simulation independently over the time framework, a GPU can prevail over a traditional CPU parallel computing where each thread may still need to loop over a large number of walkers.

[0091] Regarding example implementations according to the present disclosure, to further enhance GPU performance, several strategies can be employed. These strategies include conversion data type from double precision to single precision, utilization of shared memory to accelerate data accessing, branch reduction, loop unrolling, and others.

[0092] Several numerical tests have been done to study the GPU performance. The impact of the number of threads per block on GPU parallel computing is first evaluated. The tested example for FIGS. **11A-11B** is a single spherical pore with dimension of  $120 \times 120 \times 120$ . Image resolution, surface relaxivity, and bulk diffusion coefficient are  $0.1 \mu\text{m}$ ,  $20 \mu\text{m/s}$ , and  $2500 \mu\text{m}^2/\text{s}$ , respectively. A no-flux boundary condition is applied, and the total number of walkers is fixed to 100000. The tested example for FIG. **11C** is a Berea sandstone. The image dimension and resolution are  $256 \times 256 \times 256$  and  $2.7745 \mu\text{m}$ . All the other settings are the same as the above test.

[0093] FIGS. **11A-11C** are graphs that show GPU performance in executing the NMR numerical simulations according to the present disclosure. FIG. **11A** shows a graph **1100** that shows an estimated elapsed time under different numbers of threads per block. Graph **1100** includes x-axis **1102** of threads per block and y-axis **1104** of elapsed time (in seconds). Curve **1106** connects values that represent a number of blocks within the grid for each number of threads per block.

[0094] FIG. **11B** shows a graph **1130** that shows an estimated elapsed time under different numbers of walkers. Graph **1130** includes x-axis **1132** of walker numbers and y-axis **1134** of elapsed time (in seconds). Curve **1136** connects values that represent a number of blocks within the grid for each number of walkers (from 10,000 to 640,000).

[0095] FIG. **11C** shows a graph **1160** that shows an estimated elapsed time under different GPUs tested on the method **300** according to the present disclosure. Graph **1160** includes x-axis **1162** of GPU type (five tested) and y-axis **1164** of elapsed time (in seconds). Details of each GPU type are shown in Table **1500** of FIG. **15**. Curve **1166** connects values that represent a number of blocks within the grid for each GPU type. As shown in these graphs, when the number of threads is 128, the performance of method **300**, tested on NVIDIA RTX A6000, is optimized with a good balance of computing and memory throughput and relatively high GPU utilization. For the following tests, the number of threads per block is fixed to 128

[0096] These graphs show the results of GPU scalability performance that was studied in implementing method **300**. All the simulation settings remained unchanged except the number of walkers (which doubles). As a result, the number of blocks per the grid doubles as well with the number of threads per block fixed. Graph **1130** shows the elapsed time for the tested cases. When the number of walkers is greater than 160,000, the simulation time starts to linearly scale with the number of walkers. Thus, the GPU is keeping busy even though the GPU is not fully utilized (in other words, occupancy is not 100%). It can be important, in some aspects, to increase the GPU utilization so that an increasing number of threads can participate in parallel computing.

[0097] In addition, a crosswise evaluation is conducted to compare the performance of different GPUs as shown in graph **1160**. Graph **1160** shows elapsed time of random walk simulation running on five NVIDIA GPUs (with details listed in Table **1500** as noted). However, the parameters of each example GPU in Table **1500** does not mean that the GPU performance only depends on these parameters. Generally, with respect to the implementation of method **300**, GPU parallel computing exhibits a better performance if the GPU has a larger number of CUDA cores, higher bandwidth and TFLOPS. This can explain why the elapsed times on A40 and RTX A6000 are very close (since

they have very similar specifications). On the other hand, the current setting to achieve the optimal performance of RTX A6000 may not achieve the exact same results for other GPUs.

[0098] In addition to testing the processes (including method **300**) of the present disclosure on various GPUs, testing of the accuracy and efficiency of a validated commercial software, namely PerGeos, was performed. Three examples in the PerGeos tests were considered, including a spherical pore, a Berea sandstone, and an Estailades limestone. These examples are shown in FIG. **12**, which shows a schematic diagram **1200** that shows a comparison of NMR numerical simulations of different examples. In the diagram **1200**, (a) represents the spherical pore with dimensions of  $120 \times 120 \times 120$  and image resolution of  $0.1 \mu\text{m}$ . In the diagram **1200**, (b) represents the Berea sandstone with dimensions of  $256 \times 256 \times 256$  and image resolution of  $2.7745 \mu\text{m}$ . In the diagram **1200**, (c) represents the Estailades limestone with dimensions of  $512 \times 512 \times 512$  and image resolution of  $3.3114 \mu\text{m}$ .

[0099] FIG. **13** represents the results (in graph **1300**) that compares the efficiency of implementations of a GPU executing the NMR numerical simulations according to the present disclosure (with results **1308**) with the PerGeos software simulations (with results **1306**). Graph **1300** includes x-axis **1302** that represents digital rock type (spherical pore, Berea sandstone, or Estailades) and y-axis **1304** that represents elapsed time (in seconds). For PerGeos, two simulations for each example were executed: one using one CPU and the other one using four CPUs. The elapsed time for one- and four-CPU scenarios are displayed outside and inside the bracket, respectively, shown above each bar that represents the results **1306** for PerGeos. It is observed that a GPU executing the NMR numerical simulations according to the present disclosure achieves approximately 88 times, 29 times, and 55 times speedup at maximum for simulation in spherical pore, Berea sandstone, and Estailades limestone, respectively.

[0100] FIG. **14** represents the results (in graph **1400**) that compares the accuracy of implementations of a GPU executing the NMR numerical simulations according to the present disclosure (with results **1408**) with the PerGeos software simulations (with results **1406**). Graph **1400** includes x-axis **1402** of time (in ms) and a y-axis **1404** of normalized amplitude of NMR T.sub.2 relaxation. Three curves (one for each of the spherical pore, Berea sandstone, and Estailades limestone) are shown for both the results **1408** for a GPU executing the NMR numerical simulations according to the present disclosure and the results **1406** for the PerGeos software simulations. As shown, there is an accuracy discrepancy between the results **1408** and the results **1406** (with the results for the spherical pore highlighted in the inset of the graph **1400**).

[0101] FIG. **16** shows a schematic drawing of a control system **1600** that can be used to implement one or more processes described in the present disclosure. Some or all of the example control system **1600** can be implemented as cloud-based system and/or service, alone or in combination with other portions of the example control system **1600**. The controller **1600** is intended to include various forms of digital computers, such as printed circuit boards (PCB), processors, digital circuitry, or otherwise. Additionally, the system can include portable storage media, such as, Universal Serial Bus (USB) flash drives. For example, the USB flash drives may store operating systems and other applications. The USB flash drives can include input/output components, such as a wireless transmitter or USB connector that may be inserted into a USB port of another computing device.

[0102] The controller **1600** includes a processor **1610**, a memory **1620**, a storage device **1630**, and an input/output device **1640**. Each of the components **1610**, **1620**, **1630**, and **1640** are interconnected using a system bus **1650**. The processor **1610** is capable of processing instructions for execution within the controller **1600**. The processor may be designed using any of a number of architectures. For example, the processor **1610** may be a CISC (Complex Instruction Set Computers) processor, a RISC (Reduced Instruction Set Computer) processor, or a MISC (Minimal Instruction Set Computer) processor.

[0103] In one implementation, the processor **1610** is a single-threaded processor. In another

implementation, the processor **1610** is a multi-threaded processor. The processor **1610** is capable of processing instructions stored in the memory **1620** or on the storage device **1630** to display graphical information for a user interface on the input/output device **1640**.

[0104] The memory **1620** stores information within the control system **1600**. In one implementation, the memory **1620** is a computer-readable medium. In one implementation, the memory **1620** is a volatile memory unit. In another implementation, the memory **1620** is a non-volatile memory unit.

[0105] The storage device **1630** is capable of providing mass storage for the controller **1600**. In one implementation, the storage device **1630** is a computer-readable medium. In various different implementations, the storage device **1630** may be a floppy disk device, a hard disk device, an optical disk device, a tape device, flash memory, a solid state device (SSD), or a combination thereof.

[0106] The input/output device **1640** provides input/output operations for the controller **1600**. In one implementation, the input/output device **1640** includes a keyboard and/or pointing device. In another implementation, the input/output device **1640** includes a display unit for displaying graphical user interfaces.

[0107] The features described can be implemented in digital electronic circuitry, or in computer hardware, firmware, software, or in combinations of them. The apparatus can be implemented in a computer program product tangibly embodied in an information carrier, for example, in a machine-readable storage device for execution by a programmable processor; and method steps can be performed by a programmable processor executing a program of instructions to perform functions of the described implementations by operating on input data and generating output. The described features can be implemented advantageously in one or more computer programs that are executable on a programmable system including at least one programmable processor coupled to receive data and instructions from, and to transmit data and instructions to, a data storage system, at least one input device, and at least one output device. A computer program is a set of instructions that can be used, directly or indirectly, in a computer to perform a certain activity or bring about a certain result. A computer program can be written in any form of programming language, including compiled or interpreted languages, and it can be deployed in any form, including as a stand-alone program or as a module, component, subroutine, or other unit suitable for use in a computing environment.

[0108] Suitable processors for the execution of a program of instructions include, by way of example, both general and special purpose microprocessors, and the sole processor or one of multiple processors of any kind of computer. Generally, a processor will receive instructions and data from a read-only memory or a random access memory or both. The essential elements of a computer are a processor for executing instructions and one or more memories for storing instructions and data. Generally, a computer will also include, or be operatively coupled to communicate with, one or more mass storage devices for storing data files; such devices include magnetic disks, such as internal hard disks and removable disks; magneto-optical disks; and optical disks. Storage devices suitable for tangibly embodying computer program instructions and data include all forms of non-volatile memory, including by way of example semiconductor memory devices, such as EPROM, EEPROM, solid state drives (SSDs), and flash memory devices; magnetic disks such as internal hard disks and removable disks; magneto-optical disks; and CD-ROM and DVD-ROM disks. The processor and the memory can be supplemented by, or incorporated in, ASICs (application-specific integrated circuits).

[0109] To provide for interaction with a user, the features can be implemented on a computer having a display device such as a CRT (cathode ray tube) or LCD (liquid crystal display) or LED (light-emitting diode) monitor for displaying information to the user and a keyboard and a pointing device such as a mouse or a trackball by which the user can provide input to the computer.

Additionally, such activities can be implemented via touchscreen flat-panel displays and other

appropriate mechanisms.

[0110] The features can be implemented in a control system that includes a back-end component, such as a data server, or that includes a middleware component, such as an application server or an Internet server, or that includes a front-end component, such as a client computer having a graphical user interface or an Internet browser, or any combination of them. The components of the system can be connected by any form or medium of digital data communication such as a communication network. Examples of communication networks include a local area network (“LAN”), a wide area network (“WAN”), peer-to-peer networks (having ad-hoc or static members), grid computing infrastructures, and the Internet.

[0111] While this specification contains many specific implementation details, these should not be construed as limitations on the scope of any inventions or of what may be claimed, but rather as descriptions of features specific to particular implementations of particular inventions. Certain features that are described in this specification in the context of separate implementations can also be implemented in combination in a single implementation. Conversely, various features that are described in the context of a single implementation can also be implemented in multiple implementations separately or in any suitable subcombination. Moreover, although features may be described above as acting in certain combinations and even initially claimed as such, one or more features from a claimed combination can in some cases be excised from the combination, and the claimed combination may be directed to a subcombination or variation of a subcombination.

[0112] Similarly, while operations are depicted in the drawings in a particular order, this should not be understood as requiring that such operations be performed in the particular order shown or in sequential order, or that all illustrated operations be performed, to achieve desirable results. In certain circumstances, multitasking and parallel processing may be advantageous. Moreover, the separation of various system components in the implementations described above should not be understood as requiring such separation in all implementations, and it should be understood that the described program components and systems can generally be integrated together in a single software product or packaged into multiple software products.

[0113] A number of implementations have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the disclosure. For example, example operations, methods, or processes described herein may include more steps or fewer steps than those described. Further, the steps in such example operations, methods, or processes may be performed in different successions than that described or illustrated in the figures. Accordingly, other implementations are within the scope of the following claims.

## Claims

1. A computer-implemented method of resolving a surface roughness effect with a GPU-accelerated NMR simulation, comprising: identifying, with a graphics processing unit (GPU), a segmented micro-CT image input as a computational domain; assigning, with the GPU, a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating, with the GPU, a random walk numerical simulation with the plurality of random walkers; moving, with the GPU, each random walker of the plurality of random walkers from a previous position to a new position; determining, with the GPU, the new position of each random walker; and updating, with the GPU, an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.
2. The computer-implemented method of claim 1, wherein determining the new position of each random walker comprises determining, with the GPU, that the new position is a pore voxel, with an NMR magnetization of the random walker staying the same with no decline.
3. The computer-implemented method of claim 2, wherein determining the new position of each random walker comprises determining, with the GPU, that the new position is beyond the

computational domain, the method comprising: assigning, with the GPU, the random walker back to a pore voxel or the new position based on a determined boundary condition.

**4.** The computer-implemented method of claim 3, wherein the determined boundary condition is one of a no-flux boundary condition, a periodic boundary condition, or a mirror boundary condition, the method comprising assigning, with the GPU, the random walker to the new position based on the determined boundary condition and a distance that the random walker travels along an incident angle.

**5.** The computer-implemented method of claim 3, wherein determining the new position of each random walker comprises determining, with the GPU, that the new position is a solid voxel, the method comprising: updating, with the GPU, a decline factor to the NMR magnetization of the random walker.

**6.** The computer-implemented method of claim 5, wherein updating the NMR relaxation rate to resolve the surface roughness effect based on the new position of each random walker comprises: determining, with the GPU, a surface relaxivity strength for each of the plurality of random walkers based on a spatial heterogeneity of surface relaxivity; and assigning, with the GPU, a relaxation correction factor for each of the plurality of random walkers based on an irregularity of pore geometry.

**7.** The computer-implemented method of claim 6, further comprising adjusting, with the GPU, the NMR relaxation rate with the relaxation correction factor.

**8.** The computer-implemented method of claim 1, wherein a number of the plurality of random walkers is up to a maximal number of active threads on the GPU based at least in part on a GPU specification and GPU utilization.

**9.** A graphics processing unit (GPU), comprising: a plurality of CUDA cores; and at least one memory module configured to store a plurality of instructions that, when executed by the plurality of CUDA cores, causes the plurality of CUDA cores to perform operations, comprising: identifying a segmented micro-CT image input as a computational domain; assigning a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating a random walk numerical simulation with the plurality of random walkers; moving each random walker of the plurality of random walkers from a previous position to a new position; determining the new position of each random walker; and updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.

**10.** The GPU of claim 9, wherein the operation of determining the new position of each random walker comprises determining that the new position is a pore voxel, with an NMR magnetization of the random walker staying the same with no decline.

**11.** The GPU of claim 10, wherein the operation of determining the new position of each random walker comprises determining that the new position is beyond the computational domain, and the operations further comprise: assigning the random walker back to a pore voxel or the new position based on a determined boundary condition.

**12.** The GPU of claim 11, wherein the determined boundary condition is one of a no-flux boundary condition, a periodic boundary condition, or a mirror boundary condition, and the operations further comprise assigning the random walker to the new position based on the determined boundary condition and a distance that the random walker travels along an incident angle.

**13.** The GPU of claim 11, wherein the operation of determining the new position of each random walker comprises determining that the new position is a solid voxel, and the operations further comprise: updating a decline factor to the NMR magnetization of the random walker.

**14.** The GPU of claim 13, wherein the operation of updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker comprises: determining a surface relaxivity strength for each of the plurality of random walkers based on a spatial heterogeneity of surface relaxivity; and assigning a relaxation correction factor for each of the plurality of random walkers based on an irregularity of pore geometry.

- 15.** The GPU of claim 14, wherein the operations comprise adjusting the NMR relaxation rate with the relaxation correction factor.
- 16.** The GPU of claim 9, wherein a number of the plurality of random walkers is up to a maximal number of active threads on the GPU based at least in part on a GPU specification and GPU utilization.
- 17.** An apparatus comprising a tangible, non-transitory computer-readable memory that stores instructions executable by a graphics processing unit (GPU) to perform operations, comprising: identifying a segmented micro-CT image input as a computational domain; assigning a plurality of random walkers into pore voxels of the segmented micro-CT image; initiating a random walk numerical simulation with the plurality of random walkers; moving each random walker of the plurality of random walkers from a previous position to a new position; determining the new position of each random walker; and updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker.
- 18.** The apparatus of claim 17, wherein the operation of determining the new position of each random walker comprises determining that the new position is a pore voxel, with an NMR magnetization of the random walker staying the same with no decline.
- 19.** The apparatus of claim 18, wherein the operation of determining the new position of each random walker comprises determining that the new position is beyond the computational domain, and the operations further comprise: assigning the random walker back to a pore voxel or the new position based on a determined boundary condition.
- 20.** The apparatus of claim 19, wherein the determined boundary condition is one of a no-flux boundary condition, a periodic boundary condition, or a mirror boundary condition, and the operations further comprise assigning the random walker to the new position based on the determined boundary condition and a distance that the random walker travels along an incident angle.
- 21.** The apparatus of claim 19, wherein the operation of determining the new position of each random walker comprises determining that the new position is a solid voxel, and the operations further comprise: updating a decline factor to the NMR magnetization of the random walker.
- 22.** The apparatus of claim 21, wherein the operation of updating an NMR relaxation rate to resolve a surface roughness effect based on the new position of each random walker comprises: determining a surface relaxivity strength for each of the plurality of random walkers based on a spatial heterogeneity of surface relaxivity; and assigning a relaxation correction factor for each of the plurality of random walkers based on an irregularity of pore geometry.
- 23.** The apparatus of claim 22, wherein the operations comprise adjusting the NMR relaxation rate with the relaxation correction factor.
- 24.** The apparatus of claim 17, wherein a number of the plurality of random walkers is up to a maximal number of active threads on the GPU based at least in part on a GPU specification and GPU utilization.
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