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Analysis and approximation of a finite-range jump process

Rich Lehoucq (SNL), Qiang Du (PSU), Max Gunzburger (FSU), Stephen Bond (SNL), Nate Burch (Gonzaga), Marta D'Elia (FSU), Zhan Huang (PSU), Scott McKinley (UF), Stephen Rowe (Texas A&M)

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Mathematical and Numerical Analysis of Peridynamics for Multiscale Problems in Solids

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Review of classical diffusion

- Observation: stuff spreads from higher to lower concentrations; typical examples include pressure, energy (heat), the spread of odor in a room, contaminant or pollutant in a lake, colored dye in water, etc.
- **microscopic model**: Brownian motion

  $$X_t = \sqrt{2D}\, W_t$$

  where W_t is a Wiener stochastic process
- **macroscopic model**: Variance of the spread of particles satisfies

  $$\mathbb{E}\, X_t^2 \propto t, \text{ e.g. }, \mathbb{E}\, X_t^2 = 2D\, t$$

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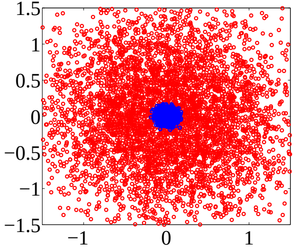
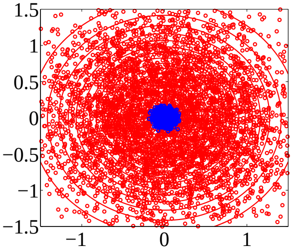
Stochastic process and deterministic counterpart (PDE)



(a) Realizations $\sqrt{2D}\,W_t$



(b) $\dfrac{\partial u}{\partial t} = \nabla \cdot D\nabla u$

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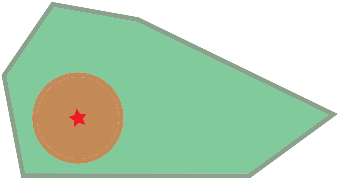
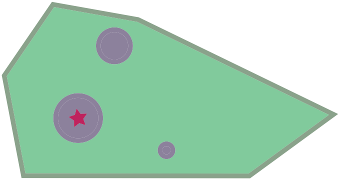
Diffusion applications

- flow through porous media; heat conduction
- spread of an invasive species, seed dispersal, disease transmission, foraging or migrating animals



In many applications, classical diffusion may not be appropriate due to

- Heterogeneity of the underlying medium
- Nonlocal dispersion, transmission mechanisms



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Anomalous diffusion as a model

- Alternative to classical diffusion when Fick's first law, e.g., the flux $D\nabla u$ is not an expedient model
- Suppose the variance

$$\mathbb{E}\, X_t^2 \propto t^\eta$$

- anomalous subdiffusion if $\eta < 1$ (not considered in this presentation; typically a non-Markov process)
- *normal* diffusion if $\eta = 1$
- anomalous superdiffusion if $\eta > 1$ (heavy tails)
- $\eta \geq 1$ the Markov process X_t may be discontinuous and so is deemed a "jump" Process (in contrast to a Wiener process that has continuous sample paths)

Ensemble averaging in phase space

- A more general diffusion equation is given by

$$u_t(x,t) = \int_{\mathbb{R}^d} \big(h(y,x,t) - h(x,y,t)\big)\, dy$$

  Nonlocal analogue of $u_t = -\nabla \cdot \mathbf{q}$
- An expression for h can be derived as an ensemble average in phase space; see *The statistical mechanical foundation of the peridynamic nonlocal continuum theory: energy and momentum conservation laws* (L. & Sears), Physical Review E, Volume 84, 031112, 2011
- **Take home message**: there is a basis for nonlocality in nonequilibrium statistical mechanics; the classical diffusion arises via assumptions (Fick's law, or assume that the sample path is continuous)

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Nonlocal convection-diffusion equation

- Classical (linear) convection-diffusion equation

$$\begin{cases} u_t = -\nabla \cdot \mathbf{q} \\ \mathbf{q} = \mathbf{b}\, u + \mathbf{A}\, \nabla u \end{cases}$$

- Can also rewrite the diffusion equation given by ensemble averaging (in the linear case) as

$$\begin{cases} u_t = \mathcal{D} \cdot \mathbf{f} \\ \mathbf{f} = \boldsymbol{\mu}\, u + \boldsymbol{\Theta}\, \mathcal{D}^* u \end{cases}$$

- $\mathcal{D}$ and $\mathcal{D}^*$ are "nonlocal" divergence and gradient operators (that are adjoints of each other); see L., Du, Gunzburger, Zhou developed this nonlocal vector calculus (2012 SIAM review paper)

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Nonlocal convection-diffusion equation

$$u_t(x,t) = \int_{\mathbb{R}^d} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy$$

- u is a probability density, concentration, population, or temperature (for a nonlocal rigid heat conductor)
- γ is a nonnegative, not necessarily symmetric dispersal kernel, i.e., $\gamma(x,y) \neq \gamma(y,x)$, and describes the mechanism "relating" x to y
- If $\gamma(x,y) = \gamma(y,x)$ then $\int_{\mathbb{R}^d} \big(u(y,t) - u(x,t)\big)\, \gamma(x,y)\, dy$ replaces the integral operator above

Diffusion balance

$$u_t(x,t) = \int_{\mathbb{R}^d} \gamma(y,x)\, u(y,t)\, dy - \int_{\mathbb{R}^d} \gamma(x,y)\, u(x,t)\, dy$$

Probabilistic interpretation:

- First integral: rate $\gamma(y,x)\, dx$ into dx from y given probability $u(y,t)\, dy$
- Second integral: rate $\gamma(x,y)\, dy$ into dy from x given the probability $u(x,t)\, dx$
- Difference in these two rates gives the rate of change of the probability $u(x,t)\, dx$
- "Nonlocal convection" associated with asymmetric rate γ

Analogous to a continuous-time Markov chain over an uncountable (continuum) state-space—this leads to Monte-Carlo realizations

Nonlocal flux

More generally, for $\Omega \subset \mathbb{R}^d$

$$\frac{d}{dt}\int_{\Omega} u(x,t)\,dx = \underbrace{\int_{\Omega}\int_{\mathbb{R}^d\setminus\Omega} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\,dy\,dx}_{\text{nonlocal flux of probability into } \Omega \text{ from } \mathbb{R}^d\setminus\Omega}$$

- $\Omega = \mathbb{R}^d$, then $\int_{\Omega} u(x,t)\,dx = 0$ so that the probability is conserved
- Equation nonlocal since Ω and $\mathbb{R}^d \setminus \Omega$ need not be in contact
- Deterministic equation for a Markov process X_t
    1. that arises as a scaling limit of iid random variables (where the variance, mean may not be defined)
    2. jump-diffusion SDE where the “jump-measure” or its mean may not be finite

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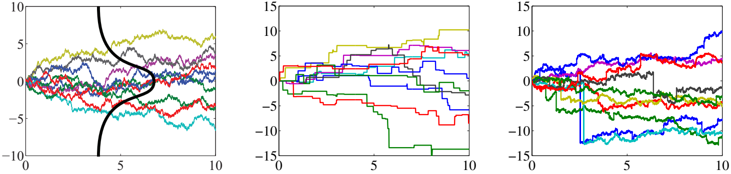
General microscopic model



(a) Wiener (b) compound Poisson (c) α-stable

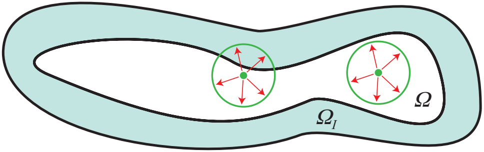
- Above examples realize a Markov process $X_t \in \mathbb{R}^d$ with translationally invariant kernels; arbitrarily large jumps possible and are examples of Lévy processes
- The case of a Wiener process is well-understood, in particular, the relationship with the PDE and on bounded domains

Our research

- Jump Markov process where the jumps are bounded "finite-range" and $X_t \in \Omega \subsetneq \mathbb{R}^d$ (on bounded domains) and their nonlocal diffusion equations with position dependent kernels
- Nonlocal variational characterization (via a nonlocal vector calculus)
  - Distinct from the classical techniques in use by the probabilistic community
  - Complimentary to fractional derivative approach
- What are the nonlocal analogue of boundary conditions? (volume-constraints!) Can show the nonlocal equations well-posed (new results)
- Discretizations of the deterministic equation are related to Monte-Carlo simulations

Formulation of volume-constrained problems

$$u_t(x,t) = \int_{\Omega \cup \Omega_{\mathcal{I}}} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy \qquad x \in \Omega$$



- $\Omega_{\mathcal{I}} = \bigcup_{x \in \Omega} B_\lambda(x)$, “interaction region”, where $B_\lambda(x)$ is the ball about x of radius $\lambda > 0$; in words, can only jump out of Ω into $\Omega_{\mathcal{I}}$
- Constraints are posed on the volume $\Omega_{\mathcal{I}} \subseteq \mathbb{R}^d \setminus \Omega$; boundary conditions may not be well-defined because sample path may jump out of Ω into $\Omega_{\mathcal{I}}$

Exit-time via the master equation

The density of particles that have not yet exited Ω to $\Omega_d \subseteq \Omega_{\mathcal{I}}$

$$\begin{cases} u_t(x,t) = \displaystyle\int_{\Omega \cup \Omega_d} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy, & x \in \Omega \\ u(x,t) = 0, & x \in \Omega_d \\ u(x,0) = u_0(x), & x \in \Omega \end{cases}$$

is used to determine the mean exit-time

$$\mathbb{E}(T) = \int_0^\infty \int_\Omega u(x,t)\, dx\, dt$$

where $T := \inf\{t : X_t \in \Omega_d \subseteq \Omega_{\mathcal{I}}\}$ is the exit-time

Mean exit-time cases

$\Omega_d \equiv \Omega_{\mathcal{I}}$

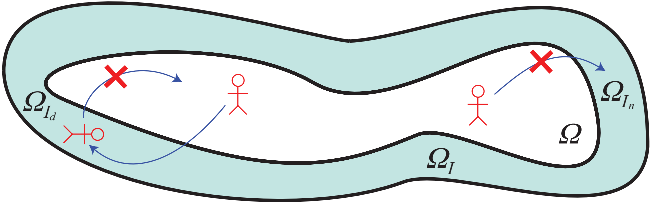
- Absorbed process with a homogenous Dirichlet volume constraint problem
- Probability is conserved over $\Omega \cup \Omega_d$, i.e., the process is either in Ω or has exited to Ω_d and has been "absorbed"

$\Omega_d \equiv \emptyset$

- Censored process with a pure Neumann volume constraint problem
- Probability is conserved over Ω , i.e., the process remains in Ω

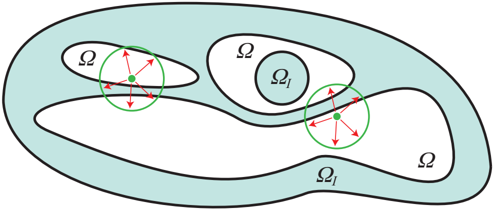
Absorbed/censored process

$\emptyset \neq \Omega_d \subsetneq \Omega_{\mathcal{I}}$ is a mixed process with a mixed volume constraint; nonlocal analogue of a mixed Dirichlet, Neumann boundary value problem



Escape probabilities

- Volume-constrained problems allow for “non-standard” domains, e.g., unconnected domains

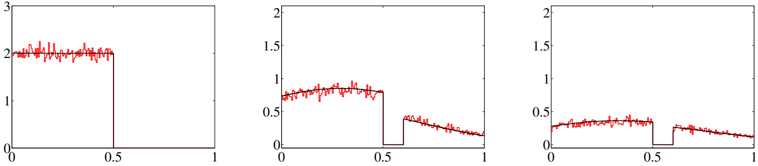


- Decomposition into escape probabilities

$$\int_{\Omega} u(x,t)\,dx = 1 - \sum_k \sum_j M_{\Omega_j}^{\Omega_{\mathcal{I}_k}}(t)$$

Escape probability example

As an illustration, consider $\Omega = (0, 0.5) \cup (0.6, 1)$ with $u_0(x) = 2 \cdot \mathbf{1}_{(0,0.5)}(x)$



(a) $t = 0.0$ (b) $t = 0.1$ (c) $t = 0.2$

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Mathematical analysis

- Goal: show that the nonlocal diffusion equation is well-posed
- Introduce a nonlocal vector calculus, an alternative to fractional derivatives
- Show that the steady-state equation is well-posed
- Standard results demonstrate that the nonlocal diffusion equation is well-posed

Nonlocal divergence

- Let $\boldsymbol{\alpha}, \mathbf{f} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3, \boldsymbol{\alpha}(x,y) = -\boldsymbol{\alpha}(y,x)$

$$\mathcal{D}(\mathbf{f})(x) := \int_{\mathbb{R}^3} \big(\mathbf{f}(x,y) + \mathbf{f}(y,x)\big) \cdot \boldsymbol{\alpha}(x,y)\, dy$$

  where $\mathcal{D}(\mathbf{f}) : \mathbb{R}^3 \to \mathbb{R}$

- $\mathcal{D}$ is a distributional divergence because

$$\boldsymbol{\alpha}(x,y) = -\frac{\partial}{\partial y}\delta(y-x) \Longrightarrow \mathcal{D}(\mathbf{f})(x) \equiv \nabla \cdot \mathbf{f}(x,x)$$

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Related operator

- Recall that $\alpha(x, y) = -\alpha(y, x)$ and define

$$\mathcal{D}^*(u)(x, y) := -\big(u(y) - u(x)\big)\,\alpha(x, y)$$

  where $\mathcal{D}^* u : \mathbb{R} \to \mathbb{R}^3$

- $\mathcal{D}^*$ is a distributional gradient because

$$\alpha(x, y) = -\frac{\partial}{\partial y}\delta(y - x) \Longrightarrow \int_{\mathbb{R}^3} \mathcal{D}^* u\, dy = -\nabla u$$

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Adjoint nonlocal divergence operator

- *Nonlocal* Green's first identity

$$\int_\Omega v\mathcal{D}(\mathcal{D}^* u)\, dx - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathcal{D}^* v \cdot \mathcal{D}^* u \, dy dx = \int_{\mathbb{R}^3 \setminus \Omega} v \mathcal{N}(\mathcal{D}^* u)\, dx$$

- Compare with the classical version

$$\int_\Omega v \Delta u \, dx + \int_\Omega \nabla v \cdot \nabla u \, dx = \int_{\partial\Omega} v \left(\nabla u \cdot \mathbf{n}\right) dS$$

- *Nonlocal* Green's first identity implies that

$$\mathcal{D}^*(u)(x,y) := -\big(u(y) - u(x)\big)\, \alpha(x,y)$$

is the adjoint of the nonlocal divergence $\mathcal{D}$

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Nonlocal diffusion via the nonlocal calculus

$$\mathcal{L}u(x) := \int_{\Omega\cup\Omega_{\mathcal{I}}} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy \qquad x \in \Omega\cup\Omega_d$$

- Nonlocal vector calculus leads to

$$\mathcal{L} = -\mathcal{D}(\boldsymbol{\mu}\, u + \boldsymbol{\Theta}\, \mathcal{D}^*\, u)$$

  where $\boldsymbol{\Theta}\colon \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3$,
- Constitutive relation $\boldsymbol{\mu}\, u + \boldsymbol{\Theta}\, \mathcal{D}^*\, u$ is a nonlocal Fick's law; $\gamma, \boldsymbol{\mu}, \boldsymbol{\Theta}$ can be of compact support
- No need for Fourier transforms as in fractional derivative approach; nonlocal vector calculus and fractional derivative approaches equivalent when the kernel is translation invariant over $\mathbb{R}^d$ and $\Omega = \mathbb{R}^d$

Nonlocal volume-constrained problem

$$\begin{cases} -\mathcal{L}u = b & \text{on } \Omega \subseteq \mathbb{R}^3 \\ \mathcal{V}u = 0 & \text{on } \Omega_{\mathcal{I}} \subseteq \mathbb{R}^3 \setminus \Omega, \end{cases}$$

- Recall the interaction region $\Omega_{\mathcal{I}}$ that we'll assume is finite and consists of $\{y\colon x \in \Omega, \quad |y - x| \leq \varepsilon\}$ where ε is not necessarily small
- "Dirichlet" volume-constraint: $\mathcal{V}u = u - g$
- Volume-constraints are the nonlocal analogues of boundary conditions and are crucial for well-posedness for the nonlocal balance laws
- Nonlocal Neumann and Robin volume-constraints also possible

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Nonlocal variational problem

Let $b \in V_c^*(\Omega \cup \Omega_{\mathcal{I}})$ find $u \in V_c(\Omega \cup \Omega_{\mathcal{I}})$

$$\int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \mathcal{D}^* u \cdot \mathcal{D}^* v \, dy \, dx = \int_{\Omega} b \, v \, dx \quad \forall v \in V_c(\Omega \cup \Omega_{\mathcal{I}})$$

- double integral (Dirichlet form) is $\int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \big(u(y) - u(x)\big)\big(v(y) - v(x)\big)\gamma(x, y) \, dy \, dx$
- The function space $V_c(\Omega \cup \Omega_{\mathcal{I}})$ incorporates the volume constraint and can be identified with specific a Hilbert spaces depending on the kernel γ and constraint functional $E_c(u)$
- Well-posedness given by the Lax-Milgram theorem

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Example: γ symmetric

Let $\gamma(x, y) = 0$ for $y \in \Omega \cup \Omega_{\mathcal{I}} \setminus B_\varepsilon^x$ where
$B_\varepsilon^x := \{y \in \Omega \cup \Omega_{\mathcal{I}} \colon |y - x| \le \varepsilon\}$

Case 1: Kernel is not integrable; positive constants $s \in (0, 1)$, γ_*, and γ^*

$$\frac{\gamma_*}{|y - x|^{d+2s}} \le \gamma(x, y) \le \frac{\gamma^*}{|y - x|^{d+2s}} \qquad |y - x| \le \varepsilon$$

Case 2: Kernel is integrable; positive constants γ_1 and γ_2

$$\gamma_1 \le \int_{B_\varepsilon^x} \gamma \, dy, \qquad \int_{\Omega \cup \Omega_{\mathcal{I}}} \gamma^2 \, dy \le \gamma_2^2$$

Well-posedness

- **Case 1**: $\|u\|_{H_c^s(\Omega\cup\Omega_{\mathcal{I}})} \leq C\|b\|_{H_c^{-s}(\Omega\cup\Omega_{\mathcal{I}})}$, $s \in (0,1)$ fractional smoothing—u gains $2s$ derivatives
- **Case 2**: $\|u\|_{L_c^2(\Omega\cup\Omega_{\mathcal{I}})} \leq C\|b\|_{L_c^2(\Omega\cup\Omega_{\mathcal{I}})}$ data is not smoothed—u gains no derivatives
- Classical formulation: $\|u\|_{H_c^1(\Omega\cup\Omega_{\mathcal{I}})} \leq C\|b\|_{H_c^{-1}(\Omega\cup\Omega_{\mathcal{I}})}$ classical smoothing—u gains 2 derivatives
- Variations on **Case 2** have been considered by Emmrich & Weckner, Rossi & colleagues, Aksoylu & Parks, Aksoylu & Mengesha
- There is an equivalence between s and the activity of the process; said another way, s characterizes the sample path

Special case

- Well-posedness **Case 1** for $s \in (0, 1/2)$ is a new result and is of interest because a trace operator is not defined in these spaces (within a Hilbert space setting)
- Consider the "finite range" Riesz kernel

$$\gamma(x, y) = \frac{C_{d,s}}{|y - x|^{d+2s}} \mathbf{1}_{|y-x| \leq \varepsilon}$$

- This leads to the volume-constrained truncated fractional Laplacian problem

$$\begin{cases} -\mathcal{L}u = b & \text{on } \Omega \subseteq \mathbb{R}^3 \\ \mathcal{V}u = 0 & \text{on } \Omega_{\mathcal{I}} \subseteq \mathbb{R}^3 \setminus \Omega, \end{cases}$$

with a homogenous Dirichlet volume-constraint on a bounded domain that is well-posed

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See also

Posters by Qiang Du and Marta D'Elia that discuss analysis, numerics, optimization

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References

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- *Computing the exit-time for a symmetric finite-range jump process* (with Nate Burch), Sandia National Laboratories, Technical report SAND 2013-5008J
- *Nonlocal convection-diffusion volume-constrained problems and jump processes* (with Qiang Du, Zhan Huang), Sandia National Laboratories, Technical report SAND 2013-5008J