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Data Article

Validation data for a hybrid smoothed dissipative particle dynamics (SDPD) spatial stochastic simulation algorithm (sSSA) method

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A R T I C L E I N F O

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A B S T R A C T

We present the validation of the hybrid sSSA-SDPD method for advection-diffusion-reaction problems coupled to discrete biochemical systems, as presented in the publication "A hybrid smoothed dissipative particle dynamics (SDPD) spatial stochastic simulation algorithm (sSSA) for advection-diffusion-reaction problems" (Drawert et al., 2019). We validate 1D diffusion, and 2D diffusion cases against their analytical solutions. We present graphs and tables of data showing the error in the simulation method.

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Specifications table

Subject area	*Computational Physics, Mechanical Engineering*
More specific subject area	*SDPD, Particle-based fluid dynamics. Reaction-diffusion master equation, Discrete stochastic simulation.*
Type of data	*Table, graph, figure*
How data was acquired	*SDPD simulations were performed using LAMMPS. Validation data was generated using Matlab codes.*
Data format	*Raw and analyzed.*
Experimental factors	*The data was created by simulation using the SDPD method*
Experimental features	*The data shows diffusion dynamics in 1D and 2D domains*
Data source location	*The data was generated on computers at UCSB and UNCA*
Data accessibility	*Data can be reproduced using the Docker container, freely available at the Git repository*: https://github.com/briandrawert/hybrid_SSA_SDPD
Related research article	*B. Drawert, B. Jacob, Z. Li, T.-M. Yi, L. Petzold. A hybrid smoothed dissipative particle dynamics (SDPD) spatial stochastic simulation algorithm (sSSA) for advection-diffusion-reaction problems, Journal of Computational Physics* [1]

Value of the data

- The data provide a detailed numerical validation of the sSSA-SDPD method compared to analytic solutions for 1D and 2D diffusion problems.
- This data contain normalized average concentration profiles for 1D (transient) and 2D (steady-state) diffusion, obtained using SDPD and sSSA-SDPD methods, as well as their L2 errors, which extend the reader's understanding of the capabilities and limitations of the methods.
- Data and methods employed can be used as a benchmark for future validations and comparisons with other spatial stochastic methods, as well as other particle-based methods such as dissipative particle dynamics (DPD).

1. Data

Data provided in this article are based on computations performed applying the hybrid SDPD-sSSA method [1] to 1D and 2D diffusion problems. The dataset includes: schematics of the validation cases tested (Fig. 1a and Fig. 2a); the normalized concentration profiles (Figs. 1b, 2c and d); the level set curves of the concentration field (Fig. 2b) and the L2 errors of the simulations, compared with the analytical results at different particle arrangements (Tables 1 and 2). Additionally, a brief description of the partial differential equations (PDEs) and their analytical solutions is provided. Routines to reproduce the data are freely available at the Git repository: https://github.com/briandrawert/hybrid_SSA_SDPD.

2. Experimental design, materials, and methods

2.1. Validation for one-dimensional diffusion

The first validation case to be considered consists of the one-dimensional transient, isotropic diffusion problem. Dirichlet boundary conditions are imposed on both sides of the domain, and the initial concentration of the domain is kept as zero. The physical model of the problem is depicted in Fig. 1a. All the physical parameters are expressed in SI units.

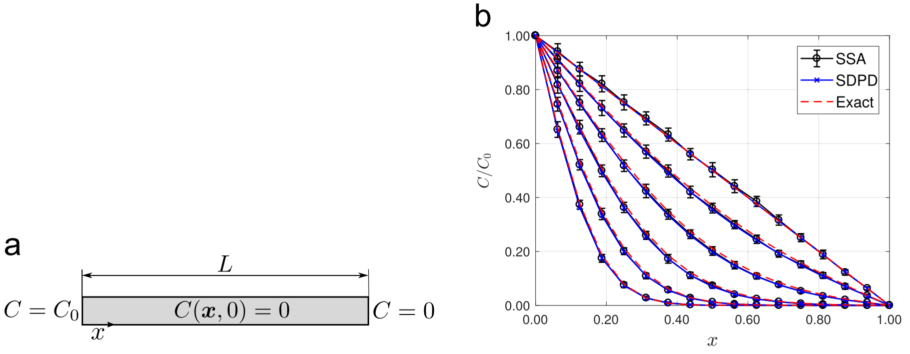

Fig. 1. (a) Schematic of diffusion in a slab, with initial and boundary conditions. (b) Comparison of profiles of the normalized concentration for selected times (bottom to top: $t = 0.01, 0.02, 0.04, 0.08, 0.16$ and $1.0[s]$).

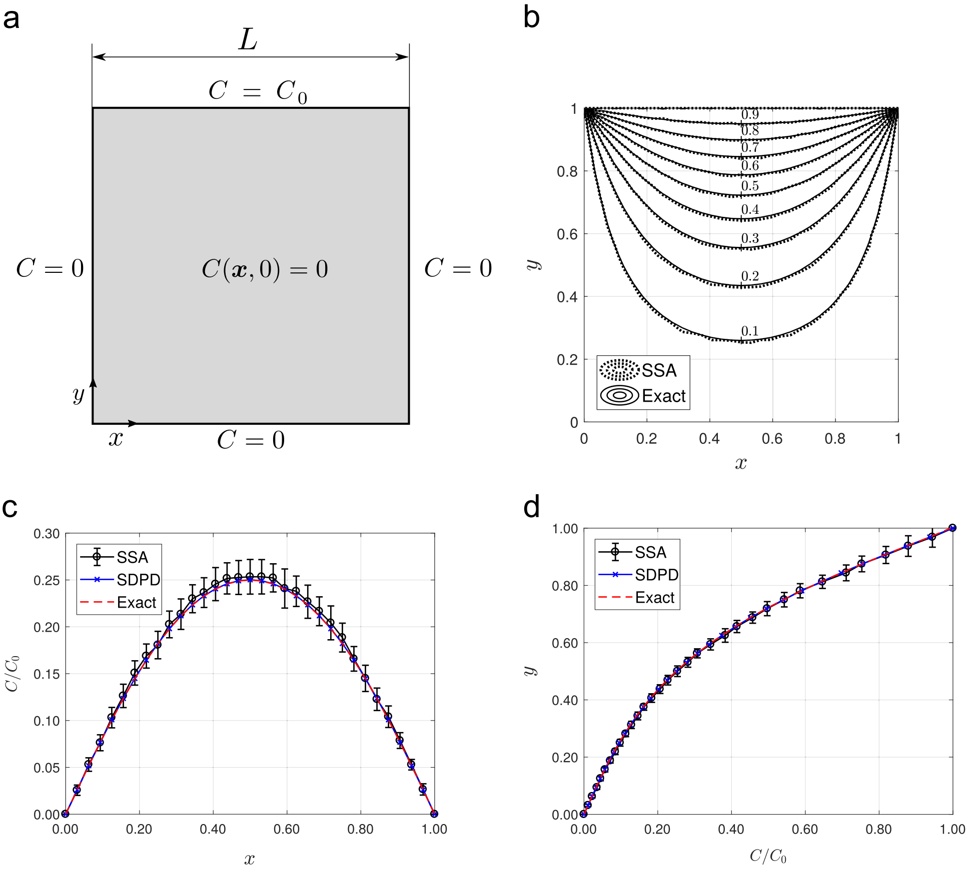

Fig. 2. (a) Schematic of diffusion in a flat plate, with initial and boundary conditions. (b) Level set curves of the normalized concentration C/C_0 at steady-state, for 33^2 particles. (c) Horizontal and (d) vertical centerline profiles of the normalized concentration at steady-state, for the case with for $N = 33^2$ particles. SSA results were averaged over $N_r = 50$ realizations.

Table 1
Results: validation of 1D transient diffusion.

Δx	N	ϵ^{SDPD} [a]	ϵ^{SSA} [b]	C_0
1/16	17	6.617×10^{-4}	8.514×10^{-4}	1.6×10^{5}
1/32	33	4.669×10^{-4}	5.278×10^{-4}	3.2×10^{5}
1/64	65	3.764×10^{-4}	8.070×10^{-4}	6.4×10^{5}

[a] Error computed at steady-state, $t = 100$.
[b] Error computed based at the mean profile of $N_r = 100$ realizations at steady-state.

The concentration of an arbitrary species $C(x,t) : [0,1] \times [0,\infty) \rightarrow R$ evolves along time in a domain $\Omega = [0.1]$. The mathematical model is given by:

$$\frac{\partial C}{\partial t} = \kappa \frac{\partial^2 C}{\partial x^2}, \tag{1}$$

with Dirichlet boundary conditions $C(0,t) = C_0$, $C(1,t) = 0$ and initial condition $C(x,0) = 0$. The initial-boundary value problem can be solved analytically, using separation of variables. The solution has the form:

$$C(x,t) = C_0(-x+1) - \sum_{n=1}^{\infty} \left(\frac{2C_0}{n\pi} \right) \sin(n\pi x) e^{-n^2\pi^2\kappa t}. \tag{2}$$

The problem is solved using both sSSA and SDPD diffusion formulations. Boundary conditions are modeled as layers of particles with fixed imposed concentrations. The mass diffusivity $\kappa = 0.1[m^2/s]$ is kept constant, and a total of three levels of refinement were used, with the distance between particles $\Delta x = 1/16$, $1/32$ and $1/64$. A time step $\Delta t = 10^{-4}[s]$ was used to ensure stability.

Due the stochastic nature of the sSSA algorithm, results were rendered as averages of multiple realizations in order to be compared with the SDPD and exact solutions. For all the three cases considered, $N_{\mathrm{r}} = 100$ realizations were performed. Hence, the sSSA results should be interpreted as first-order statistical moments, i.e., average and standard deviation.

Temporal profiles comparing sSSA and SDPD with the exact solution are shown in Fig. 1b.

Table 1 shows the quantitative results obtained. Errors ϵ^{SDPD} and ϵ^{SSA} were computed using the L^2 norm of the difference between the present method and reference solutions, normalized by the number of particles in the domain, i.e.,

$$\epsilon = \frac{\sqrt{\sum_{n=1}^{N} (C_i - C_i^{\mathrm{ref}})^2}}{C_0 N}, \tag{3}$$

where C_i^{ref} is a reference concentration, e.g., the exact solution, when available, C_0 is a normalization factor and N is the number of particles considered.

2.2. Validation for two-dimensional diffusion

The next validation case consists of a two-dimensional, steady-state, isotropic diffusion problem in a square region $\Omega = [0,1] \times [0,1]$, with a non-homogeneous Dirichlet boundary condition C_0 in the upper wall, and homogeneous conditions on the remaining boundaries, as shown in Fig. 2a. The initial condition is homogeneous, i.e., $C(\boldsymbol{x}, t=0) = 0, \ \forall \ \boldsymbol{x} \in \Omega | \boldsymbol{x} \neq \partial\Omega$. We seek to find the steady-state by evolving the problem in time until it reaches the steady-state. The mathematical model is given by

$$\frac{\partial C}{\partial t} = \kappa \nabla^2 C, \tag{4}$$

where the steady-state exact solution in known to have the form

$$C(x,y) = \sum_{n=1}^{\infty} \frac{2C_0(1-(-1)^n)}{n\pi} \frac{\sin(n\pi x)\sinh(n\pi y)}{\sinh(n\pi)}. \tag{5}$$

Table 2
Results: diffusion in a flat plate.

Δx	N	ϵ^{SDPD} [a]	ϵ^{SSA} [b]	C_0
1/16	17^2	2.337×10^{-4}	2.902×10^{-4}	2.890×10^5
1/32	33^2	5.818×10^{-5}	1.294×10^{-4}	1.089×10^6
1/64	65^2	1.438×10^{-5}	2.043×10^{-4}	4.225×10^6

[a] Error computed at steady-state, $t = 100$.
[b] Error computed based at the mean profile of $N_r = 100$ realizations at steady-state.

Simulations were performed using $17^2, 33^2$ and 65^2 equally-spaced particles distributed in a squared domain of length $L = 1$. Dirichlet boundary conditions are modeled as layers of particles with fixed imposed concentrations, avoiding the truncation of the kernel in near-boundary regions. The mass diffusivity $\kappa = 10^{-2}[m^2/s]$ is kept constant, and a time step $\Delta t = 10^{-2}[s]$ was used.

A qualitative plot of the level set curves of the normalized concentration is described by Fig. 2b. Figs. 2c–d show the horizontal and vertical centerline profiles of the normalized concentration C/C_0 at steady-state. Profiles of sSSA-resolved concentrations, along with the standard deviation bars were obtained as averages over $N_r = 50$ realizations. A list of the estimated L^2-norm errors is summarized in Table 2.

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Transparency document. Supporting Information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.103.

References

[1] B. Drawert, B. Jacob, Z. Li, T.-M. Yi, L. Petzold, A hybrid smoothed dissipative particle dynamics (SDPD) spatial stochastic simulation algorithm (sSSA) for advection-diffusion-reaction problems, J. Comput. Phys. 378 (2019) 1–17. https://doi.org/10.1016/j.jcp.2018.10.043 (1 Feb.).