Reactive Random Walk Particle Tracking (RRWPT) code

RRWPT Quick start guide

This is a code for performing reactive transport simulations in one-dimensional and two-dimensional systems. The reaction is described by A+B->P, with some rate constant *k*. The simulation is done by means of particle tracking and reduction of the mass of particles by the reaction probability. The results manifest incomplete mixing, also known as the Ovchinnikov–Zeldovich segregation phenomena. That is, the domain becomes segregated into islands where one of the species is abundant and the other is missing. As a result, the reaction slows down, in comparison with the well-mixed rate. When this happens, the concentration tends to scale like t^(-d/4) instead of scaling like t^-1 in the well-mixed solution (d is the system dimension, d=1,2,3).

Contributors

This code was written by Amir Paster, in collaboration with Diogo Bolster (ND) and David Benson (CSM).

Special thanks to Antoine Aubenau (Northwestern), Tomas Campos Aquino (ND), and the hydrology group in Notre Dame.

Citation

If you use this code, please cite our paper:
"Amir Paster, Diogo Bolster and David Benson. Particle Tracking and the Diffusion-Reaction Equation, Water Resources Research (in press)"
You may also contact us (apaster@nd.edu, or bolster@nd.edu), for updated citations.

Requirements:

-Matlab version 2012a (or higher) with Statistics toolbox

* Unfortunately, this code will only run on Matlab version 2012a (or higher), with Statistics toolbox installed. This is due to the use of the kd-tree search algorithms. If you don't have this Matlab

version, or this toolbox, you can create a work-around by using some freely available kd-tree algorithms instead (like the one by Steven Michael, in Matlab central, which we recommend). This is a rather complicated task, though, in terms of time investment in changing the code and in compiling the kd-tree mex files.

Installation & run

To run this code you need to:

1. Extract the contents of the zip file into a new folder. That folder should contain all the code.
2. Start Matlab.
3. In Matlab, change the Current Folder into the RRWPT code folder.
4. Open the main.m file in the file editor and click run (F5)

Results

If everything worked just fine, the run should be done in a few minutes.
A new subfolder (/runs/x/) will be created (x is the run number) and the following files will be stored into it:

- input.mat: contains the input parameters of the model (Matlab data file)
- log.txt: a log file of the run, containing all output sent to the screen.
- part_locX_tsi=Y.mat: a 'snapshot' of the system at a specific time. This Matlab data file contains the locations, and masses of all particles in simulation X, at time step Y.
- results.mat: Matlab data file, contains all the workspace parameters at the end of the run (input & results).

In addition, a folder for figures will be created as well. It will store the concentration figures files (if av.save_conc_plot is set to 1)

The results will also be plotted as figures -

- Fig.1 – The spatial distribution of concentration, c(x,t) vs. x.
- Fig.2 - The temporal behavior of the average concentration, <c(t)> vs. t.

Assuming everything went right, you can now start "playing" with the run parameters. You can do so in the file set_run_parameters.m. For more details, see the comments in that file.

Code Information

Code version 1.0
Code updated at Jan 4, 2013
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Contact

apaster@nd.edu, or bolster@nd.edu. Bug reports are welcome!

Sample screen shot (2D run). Each species is plotted separately.