Update for off-lattice SPPARKS model to simulate amorphous deposition for semi-conductor substrates

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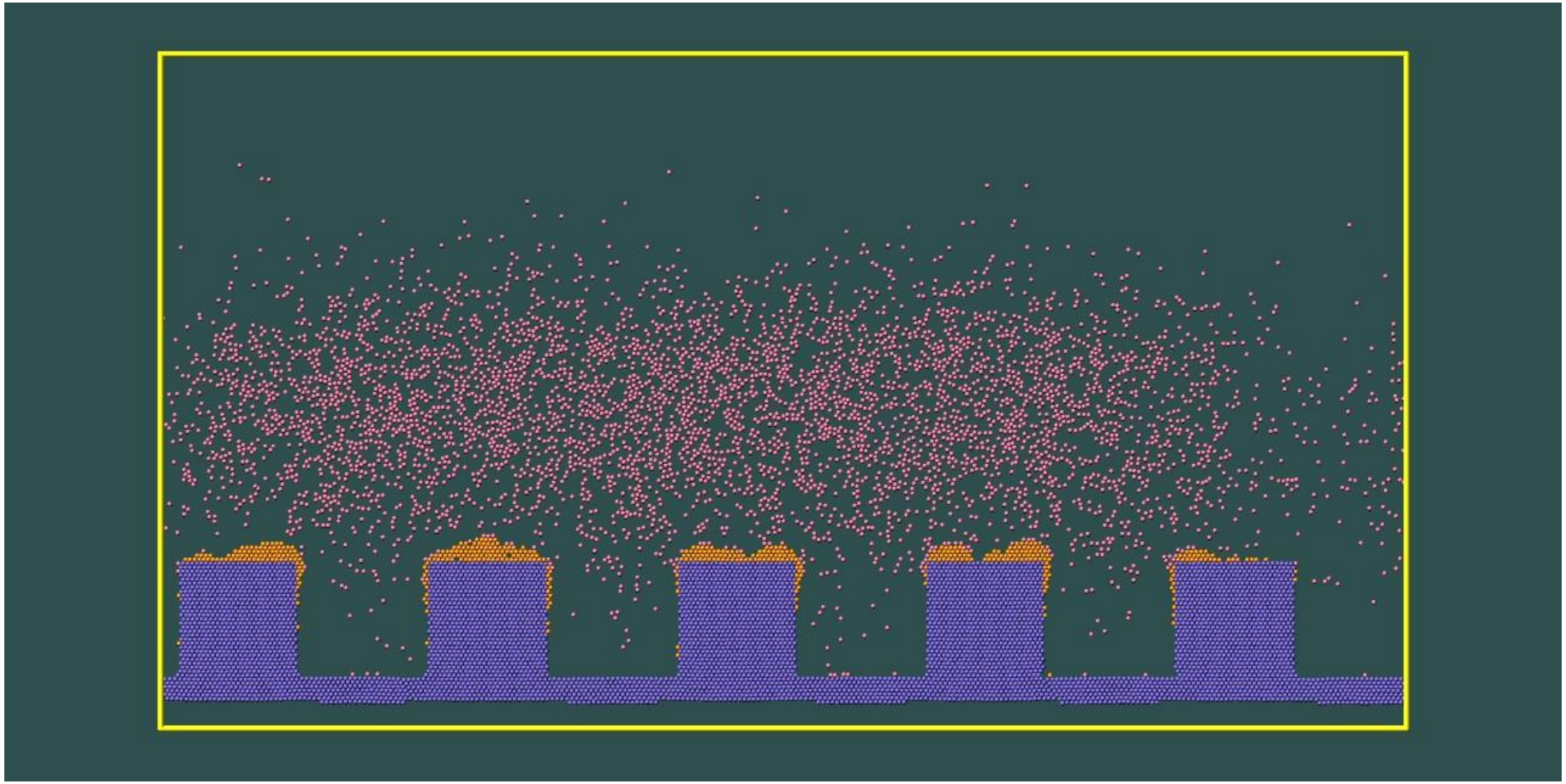
Current prototype development:

1. **Custom input file template specifies**
   - system size (2d/3d)
   - particles types/interactions
   - substrate structure
   - drift bias
   - surface reaction rate
   - visualization parameters
2. **Custom SPPARKS application ‘surfdep’**
   - added custom code to SPPARKS source
   - compiling custom code for Chemistream image
3. **Chemistream example workflow**
   - exposes simulation menu parameters
   - runs code and monitors multiple run directories
   - builds animation and displays them

Prototype model for Si deposition on a structured/rough substrate



Simple Lennard-Jones (LJ) potentials for all particle types

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

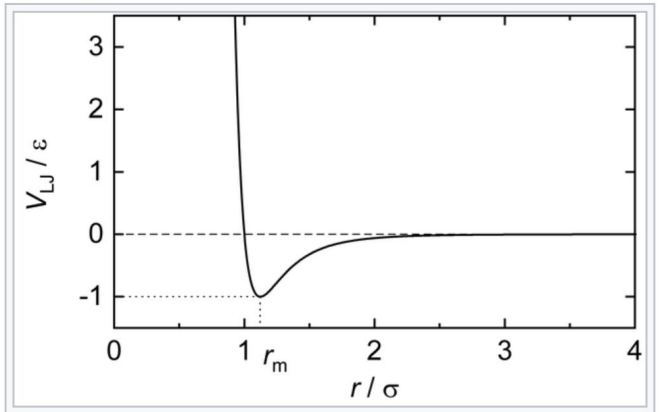


Figure 1. Graph of the Lennard-Jones potential function: Intermolecular potential energy V_{LJ} as a function of the distance of a pair of particles. The potential minimum is at $r = r_{\min} = 2^{1/6}\sigma$.

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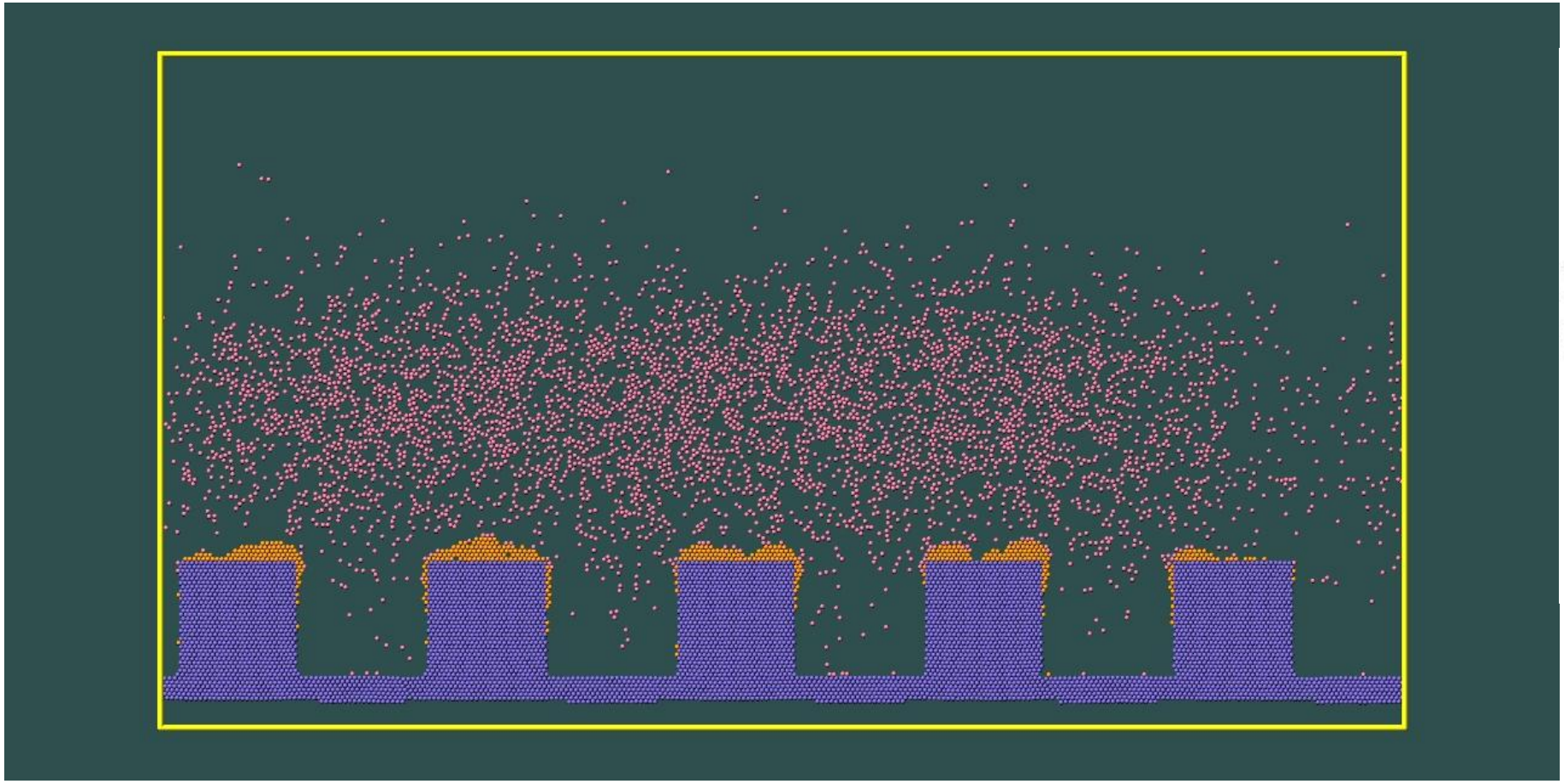

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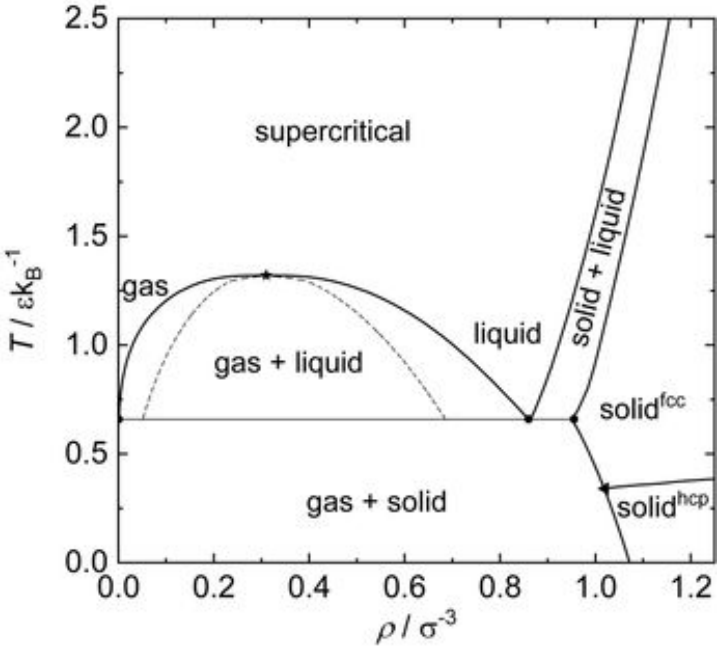

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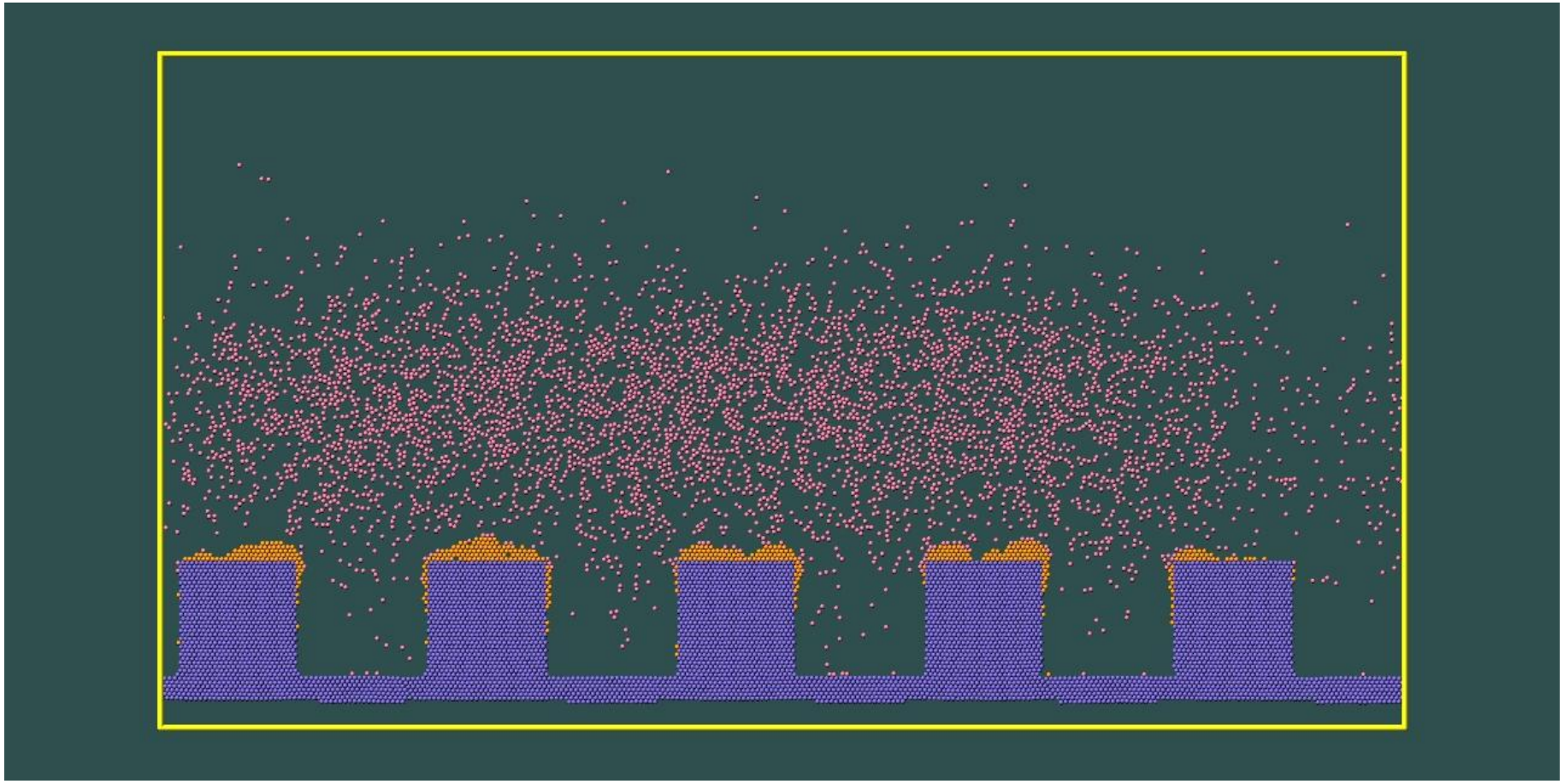

Three particle types:

- type 1: deposition species (pink)
- type 2: substrate species
- type 3: reacted/deposited species

	type_i	type_j	epsilon	sigma
pair_coeff	1	1	1.0	1.0
pair_coeff	2	2	30.0	1.0
pair_coeff	1	2	4.0	1.0
pair_coeff	3	3	30.0	1.0
pair_coeff	1	3	4.0	1.0
pair_coeff	2	3	30.0	1.0

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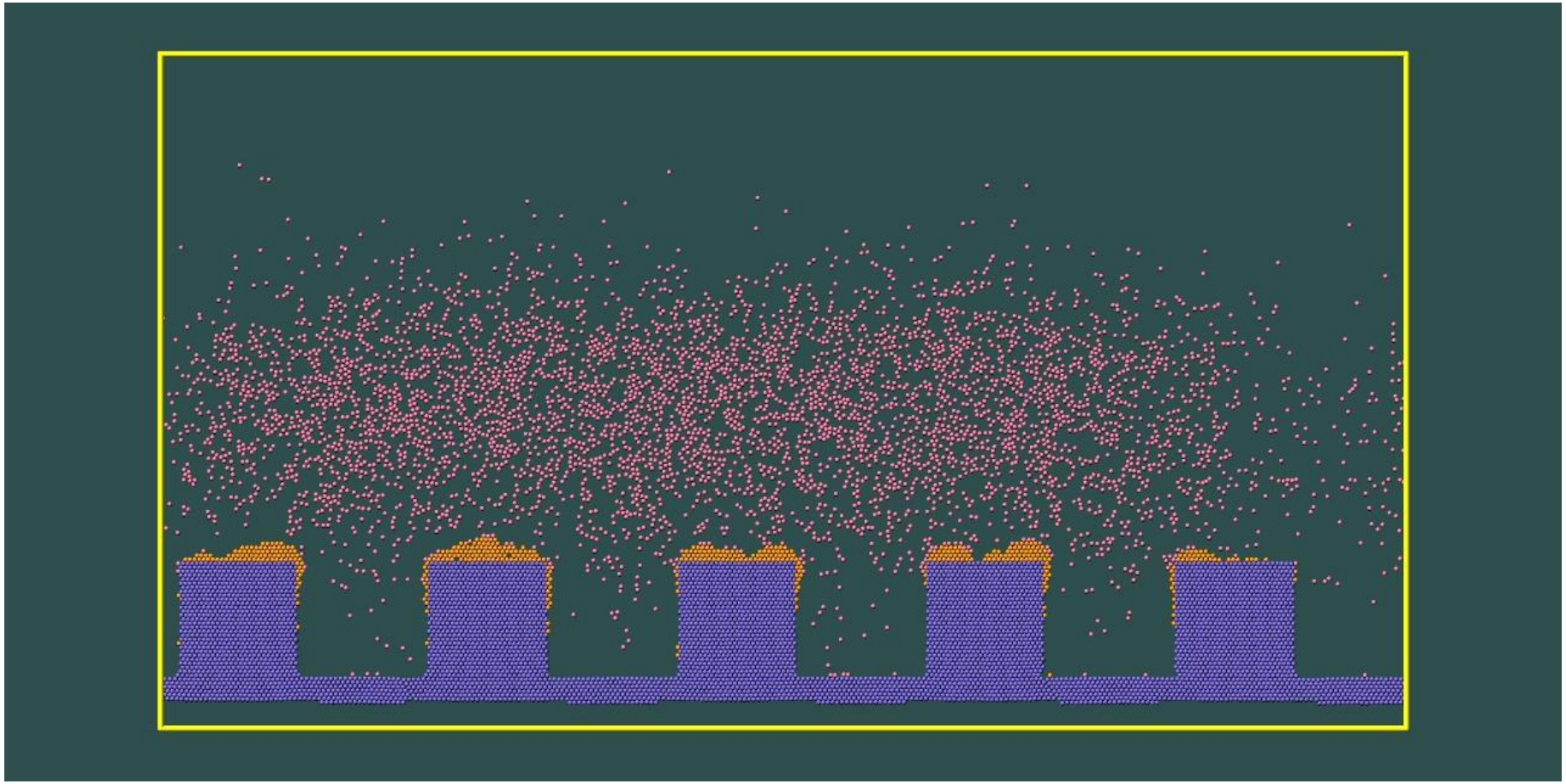

Additional model features:

- Reaction of deposition species to deposited species **type 1** → **type 3**. Based on number of substrate or deposited species particle neighbors and a user defined reaction rate
- **Imposed drift 'velocity'**, each random displacement is biased in the negative y (down) direction.
- Deposition species can **hop across the substrate surface** (can be tuned w/sigma in LJ potential

List of possible improvements

- Stillinger-Weber or Tersoff potential in SPPARKS for better treatment of Si lattice
- More realistic potentials for deposition species
- ‘Real’ small wavelength roughness??
- Expose more SPPARKS simulations parameters in Chemistream workflow
- Adjust model for deposition/reaction
  - changing cross-terms in LJ interactions
  - explicitly put rate for deposition/reaction into KMC move
- 3D parallel performance runs
- More flexible initialization for substrate and initial deposition species
- More sophisticated analysis and visualization of output
- many others possible …

What is kinetic Monte Carlo (KMC)?

- KMC simulates the time evolution of natural processes by **defining rates for events** and randomly selecting which events occur in some amount of time (time step)
- Alternative to integrating ODE or PDE kinetic equations directly
  - Allows fluctuations but algorithm is designed so that averaged quantities obey diff. eq.
  - Treats standard chemical kinetics or whatever equations are appropriate for the rates of interest (e.g., diffusion when the rates represent “hops”)
- Two main flavors
  - Rejection free: always pick some event then advance time according to the sum of all rates Q as $\Delta t = Q^{-1}\ln(1/x)$ with x a random number chosen uniformly from [0,1)
  - Rejection MC: advance time by a specified Δt and convert the list of rates to a list of probabilities for each event to happen in Δt. Random number selects whether an event happens and time advances by Δt no matter what

Thanks!