COLLISIONS AND REACTIONS

TECH-X
SIMULATIONS EMPOWERING YOUR INNOVATIONS

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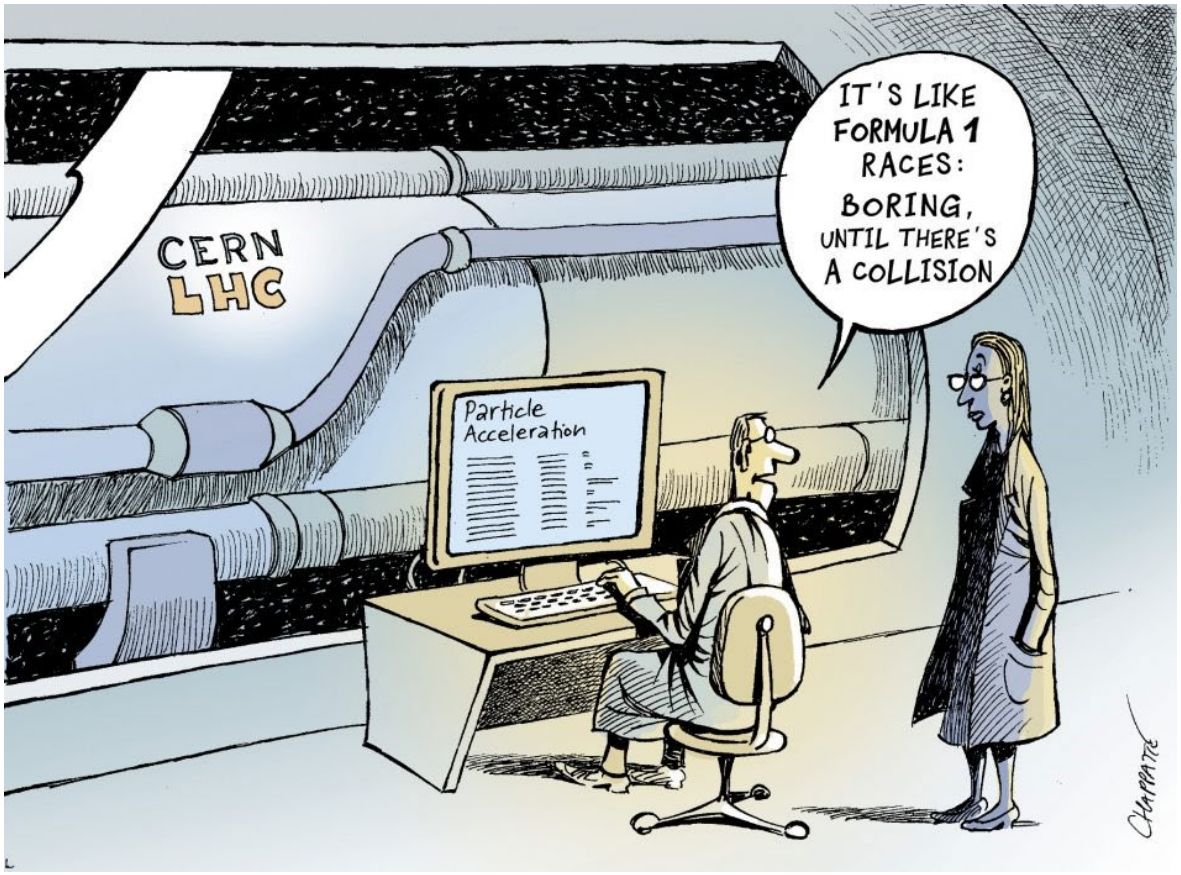
Presented by Nate Crossette



TECH-X

Talk outline

- Background on collisions
  - Basics theory
- Collision algorithms
  - General
  - New framework
- Setting up collisions
- Running with collisions

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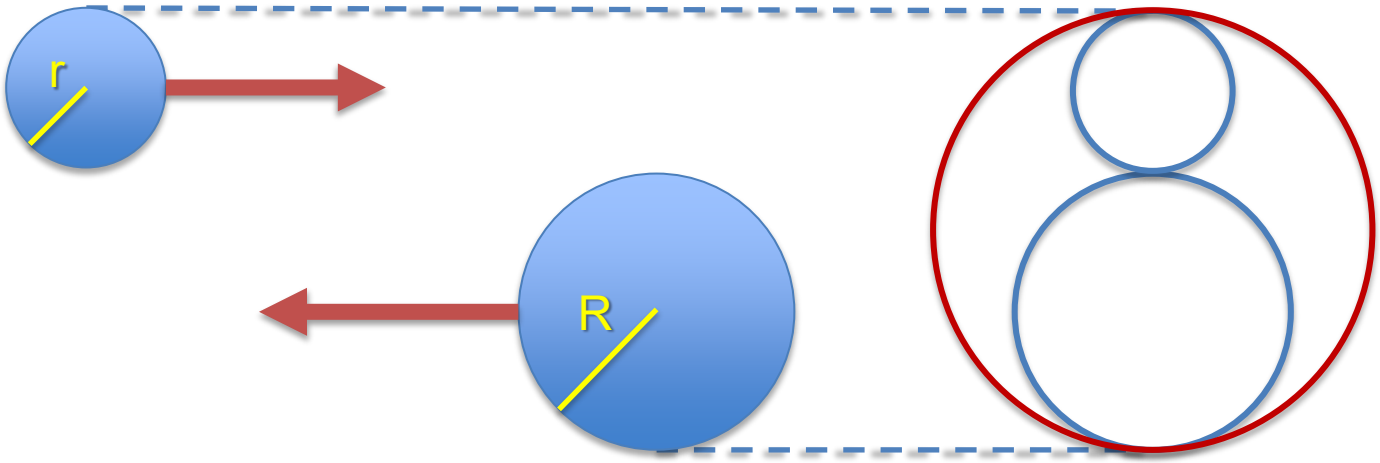
About collisions

- Can occur between one, two, three, etc reactants
- Occur on time scales not resolved by (smaller than) the simulation time step
- Can change energy, momentum, charge, and/or mass of the colliding particles

- For solid/hard objects, visualization is straightforward



The effective collision area, or cross section, is $\sigma = \pi(r + R)^2$

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Cross sections in VSim

- Cross sections are related to the rate at which collisions between two species with densities n_A and n_B take place (reactions per second per volume)

$$R = n_A n_B \langle \sigma v_{th} \rangle$$

- This can be measured experimentally for some reactions, and is also the basis for our collision algorithm in PIC codes
- Can define as a constant/function:
  - Variable hard sphere: $\sigma = \pi d^2$ where $d = d_{ref}\left(\frac{v_{ref}}{v}\right)^{\nu}$
  - Log polynomial: $\sigma = E^{-1}\left(a\, lnE + b + \frac{c}{E}\right)$
- Can be imported from a data file: LXcat – 'elec-scat'

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Probabilistic example

- Treat the collisions probabilistically
- Assume we have, in one simulation cell of size $dx = dy = dz = 1\mu$m, N=50 electrons and M=45 protons
- If we know the cross section is $\sigma = \frac{1e-15}{v}$, we can find the reaction probability for a given amount of time (lets say $\Delta t = 1\mu$s):

$$P_{rxn} = \frac{\langle \sigma v \rangle \Delta t}{V} = 0.001$$

So of NM=2250 possible reactions, 2.25 occur

But partial reactions can't occur, you say?! Indeed…

Probabilistic example (cont)

$$P_{rxn} = \frac{\langle \sigma v \rangle \Delta t}{V} = 0.001$$

- So of NM=2250 possible reactions, 2.25 occur
- Since 2.25 reactions cannot occur, we must choose 2 or 3 to occur
- On average in time we want 2.25 to occur every 1μs

- So we choose a uniformly distributed random number

$$r \in [0,1)$$

- If $r > 0.25$ we react 2 pairs, else we react 3 pairs

Probabilistic caveats

$$P_{rxn} = \frac{\langle \sigma v \rangle \Delta t}{V} = 0.001$$

- Not always constant $\langle \sigma v \rangle$, so P_{rxn} varies for each reaction pair
- Choose reaction pairs and for each one choose a random number and check against probability
- Should, on average, give the correct collision frequency
- Sensitive to number of particles per cell – more will give higher accuracy
- In VSim particles are represented as macro particles, which is accounted for.

PIC implementation

- In PIC codes, we represent many particles with a single macro particle, but the process is essentially the same for reactions

- We treat each macroparticle is a reactant, but the probability must be calculated with the true number of physical particles

$$P_{rxn} = \frac{W\sigma v\Delta t}{V}$$

weight W is physical particle per macro particle

We've selected pairs to collide, now what?

- Now we do the physics:
- General process:
  - Shift to center of momentum reference frame
  - Perform collision ensuring total momentum is zero afterwards
    - ◊ Choose angle at random (or biased), modify velocity direction
  - Shift back to lab frame

- In collisions:
  - Total energy can change (threshold energies)
  - Particles can be 'created/lost': $Ar + e^- \rightarrow Ar^+ + e^- + e^-$
  - Angular distribution can be isotropic or biased

Common collisions

- Elastic

$$A + B \rightarrow A + B$$

- Ionization/Recombination

$$A + B \leftrightarrow A^{+} + B + e^{-}$$

- Charge Exchange

$$A^{+} + B \rightarrow A + B^{+}$$

- Excitation

$$A + e \rightarrow A^{*} + e$$

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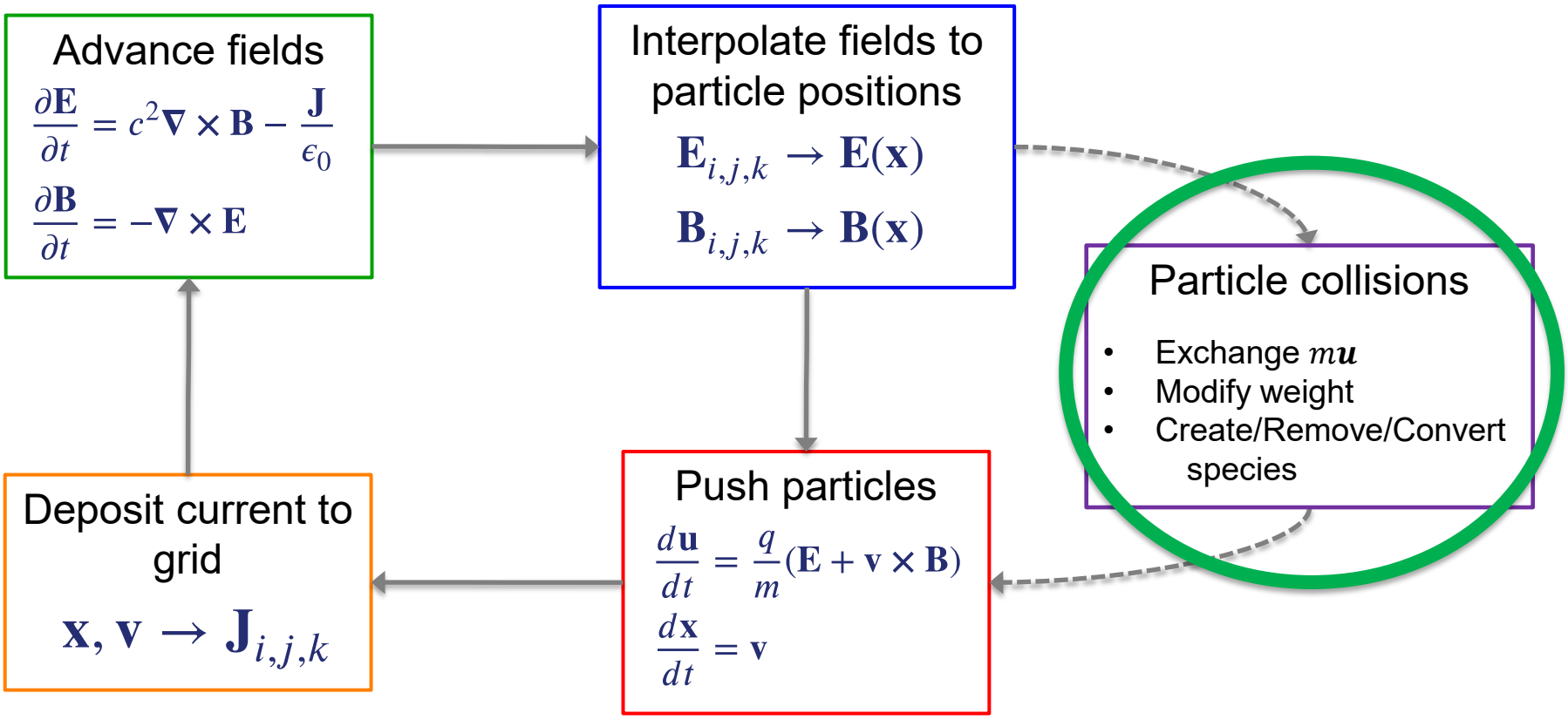
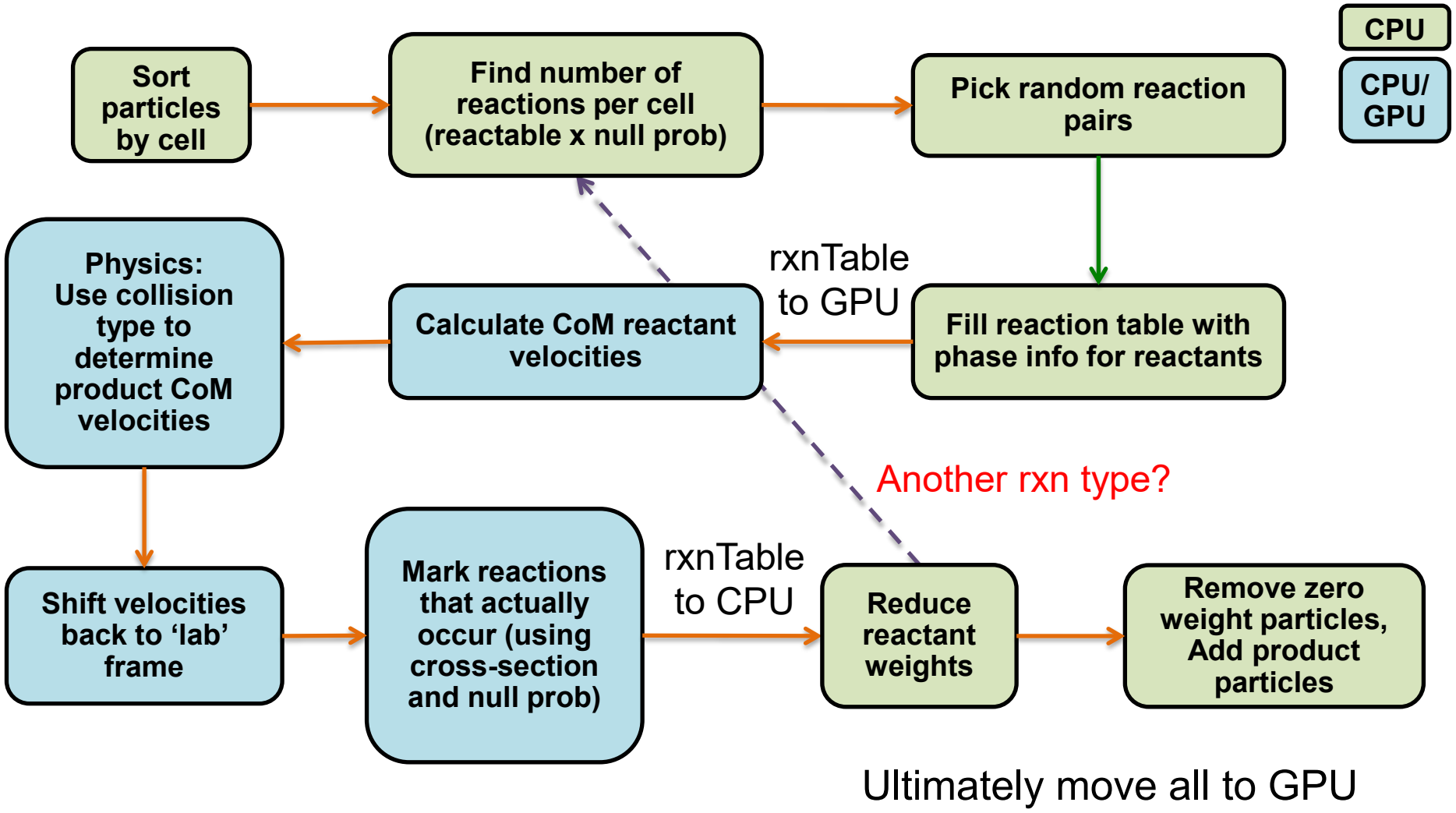
The particle-in-cell algorithm

- Macroparticles represent a large number of physical particles
- Fields on grid, particles not constrained to grid



Current reaction design



Some details

- Particles only react once per time step
  - exception being VW particles if weight > 0 after rxn
- Loop through all reaction processes (*e.g.* elastic A+B, elastic B+B, ionization C+A, etc.) in random order and update
- Particles are not removed/added until ALL reaction processes have finished updating
- This works because only a small number of particles undergo collisions in a particular time step (must be ensured by taking small enough time steps – discussed later)

Other collision improvements

N(T)C method (no time counter / null collision)[2] - Probabilistic down-selection

- Scale down number of collision pairs selected by null probability

Null probability (estimate of total probability in a cell):

$$p_{null} = \frac{\langle \sigma v \rangle_{max} \mathrm{W} \Delta t}{V}$$

Number of reaction pairs:

$$N_{RP} = {}^{1}/_{2}\, N(N-1) p_{null}$$

- For reacting, scale back up the individual reaction probability

Probability of reaction:

$$P_{rxn} = \frac{\langle \sigma v \rangle W \Delta t}{V p_{null}} = \frac{\langle \sigma v \rangle}{\langle \sigma v \rangle_{max}}$$

[2] Bird 1994 Molecular Gas Dynamics and the Direct Simulation of Gas flows

No Time Counter/Null Collision Example

$Ar + e \rightarrow A^+ + 2e$

- Say there is a cell with $\mathrm{N_{Ar}} = 20, \mathrm{N_e} = 25$.

$$\boldsymbol{N_{coll} = N_{Ar} N_e = 500}$$

- Calculate p_{null} using an estimate for $\langle \sigma v \rangle_{max}$

$$\boldsymbol{p_{null} = \frac{\langle \sigma v \rangle_{max} W \Delta t}{V} \approx .05}$$

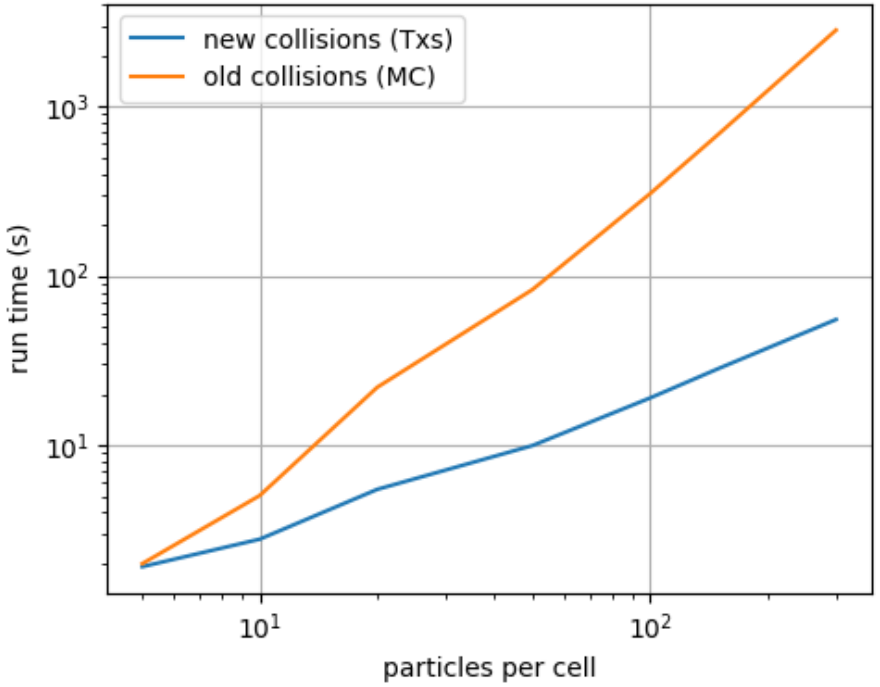
- Choose $\mathrm{N_{coll}} * p_{null} = 25$ macroparticle pairs. Then calculate upscaled probability for the 25 reactions. So, for a particular pair, the reaction probability becomes

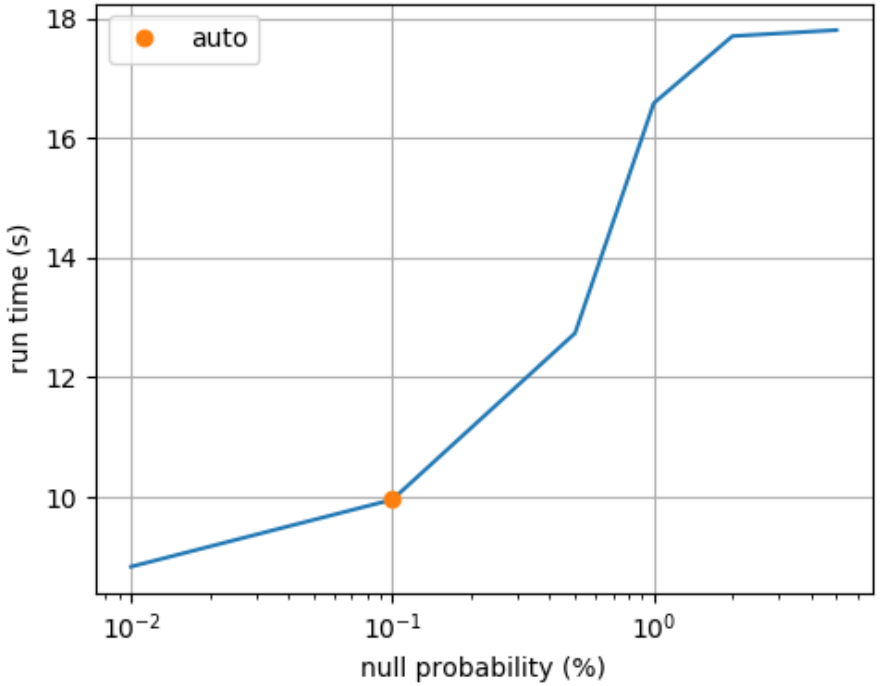
$$\boldsymbol{P_{rxn} = \frac{\langle \sigma v \rangle_{pair} W \Delta t}{V p_{null}} = \frac{p_{pair}}{p_{null}} \approx . \frac{01}{.05} = 20\%}$$

- So the particular pair has an upscaled probability of 20%.
- This means it is important to have at least 10 macroparticles per cell to get good statistics with the reactions.

Performance

- Little improvement at 5PPC, but ~2x speedup over current Vorpal at 10PPC, and >10x speedup at 100PPC





- About 2x speedup using the N(T)C method

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Not as much choice as you'd think..

- When simulating collisions we are constrained by a few choices:

- Highest density n and cross section σ give us
  - Mean free path $\lambda = \left(\sqrt{2}n\sigma\right)^{-1}$
  - Resolve mean free path, so $dx = dy = dz = \lambda/3$
  - One cell crossing, so $\Delta t = dx/(3v_{th})$

- Troubleshooting simulation with collisions – first things to check are resolution and timestep

- Remember: you ***must*** always resolve the fastest physics of import

Rxn framework .pre file

- In .pre file need:

- RxnProcess block
  - Defines reactants and products and points to rxnPhysics block

- RxnPhysics block
  - contains:
    - RxnRate block
      - Cross section kind
    - RxnProductGenerator block
      - Generator kind (elastic, ionization, etc.)

Implementation in VSim 9 text-setup

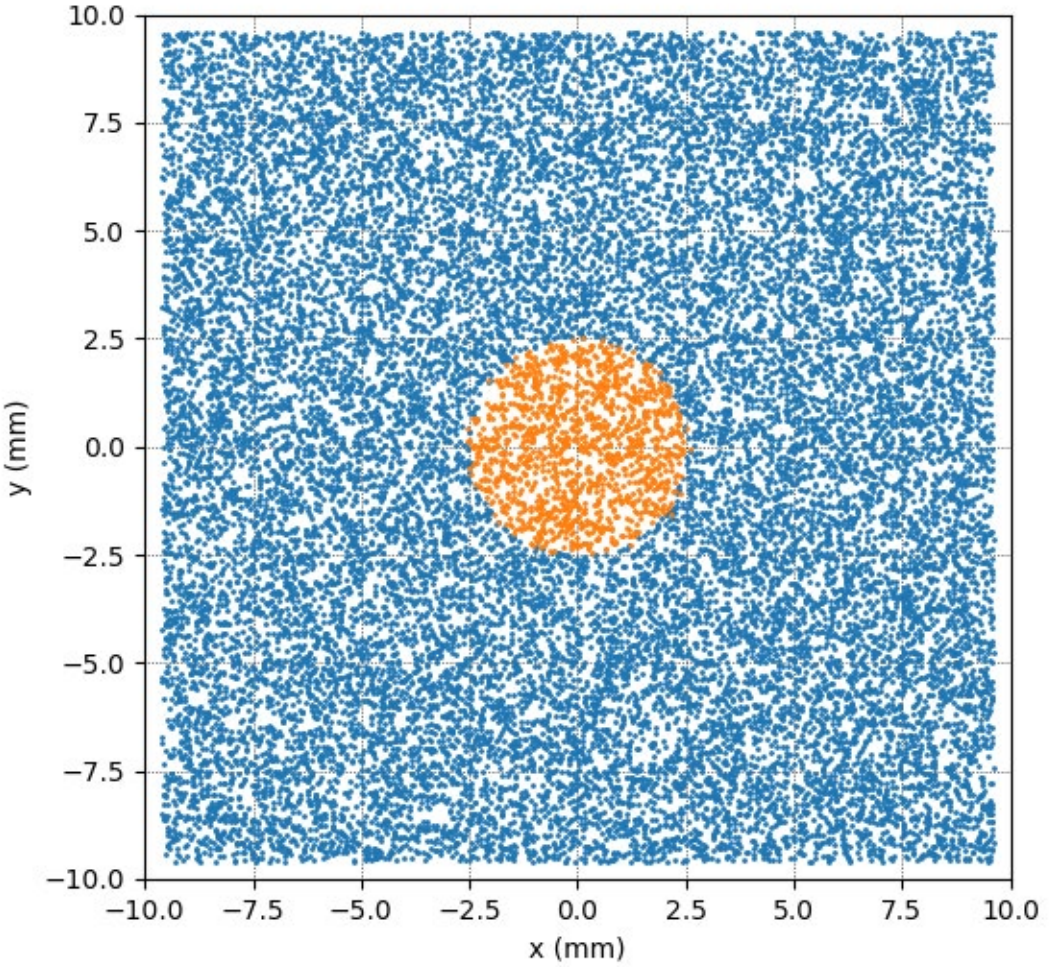
```
<RxnProcess ArEIonization>
   kind = collisionProcess
   rxnPhysics = impactIonization
   numUpdateSteps = 1
   randomSeed = 399
   reactants = [Argon Electron]
   products  = [Argon1 Electron Electron]
</RxnProcess>

<RxnPhysics impactIonization>
   kind = generalCollision
   <RxnRate rxnRate>
     kind = powerLawCrossSection
     coefficient = $PI * pow(DREF,2) * pow(VREF,2.*NU)$
     exponent = $-2.*NU$
     variable="velocity"
   </RxnRate>
  <RxnProductGenerator productGenerator>
    kind = electronIonization
    thresholdEnergy = 15.75 #eV
    randomSeed = 828
  </RxnProductGenerator>
</RxnPhysics>
```

```
##########################################
###  Field Ionization: N1 -> N2  ###
##########################################
<RxnProcess N1Ionization>
   kind = collisionProcess
   rxnPhysics = fieldIonizationN1N2
   numUpdateSteps = 1
   randomSeed = 399
   reactants = [N1 yeeEmField.edgeE]
   products  = [N2 ionizedElectrons JDep]
</RxnProcess>

<RxnPhysics fieldIonizationN1N2>
   kind = generalCollision
   <RxnRate rxnRate>
     kind = fieldIonizationDCADK
     ionizationEnergy = 29.6013
     charge = 1
   </RxnRate>
  <RxnProductGenerator productGenerator>
    kind = fieldIonization
    randomSeed = 401
  </RxnProductGenerator>
</RxnPhysics>
```

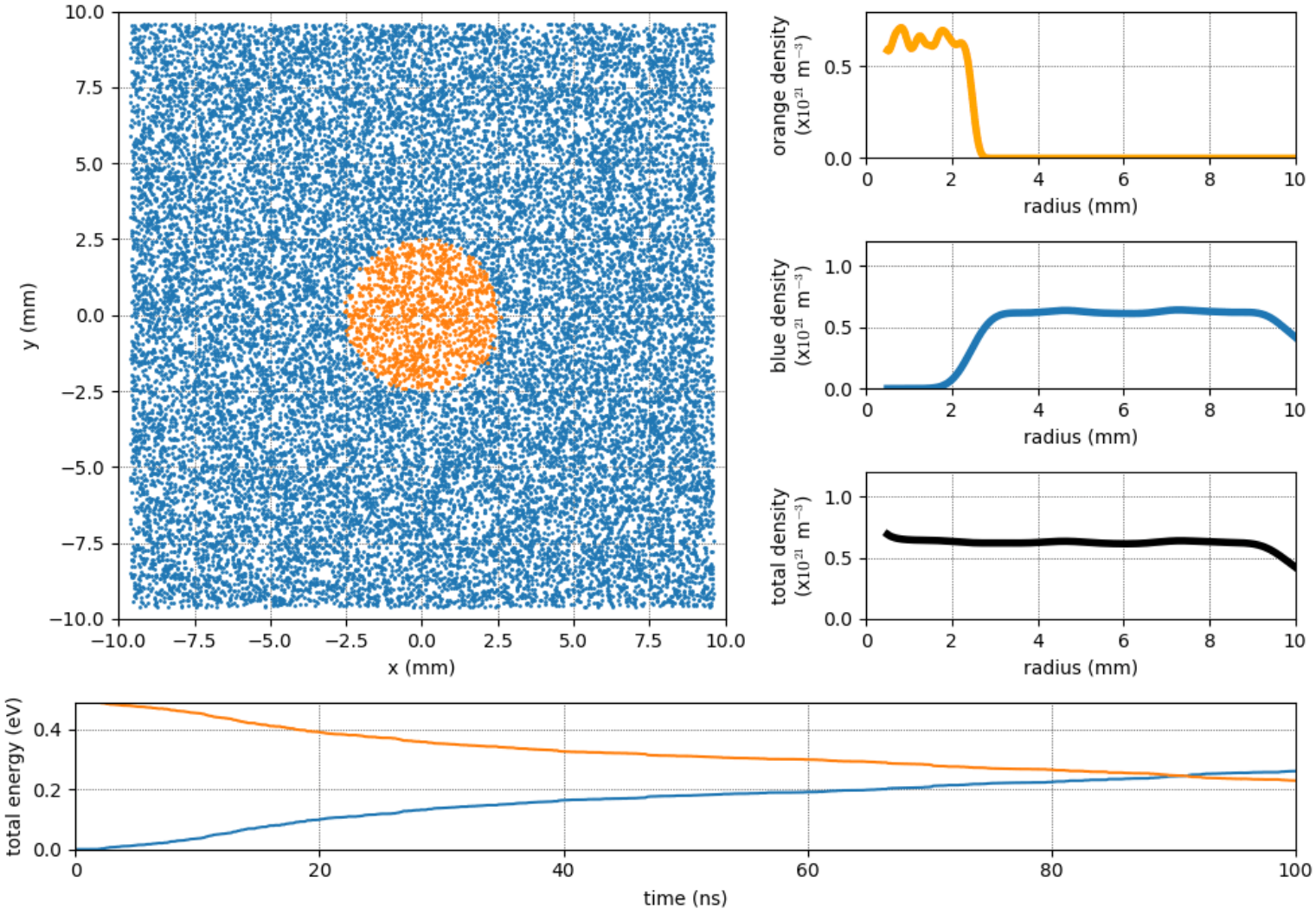
```
<RxnProcess elasticGreenRed>
  kind = collisionProcess
  rxnPhysics = elasticCollide
  numUpdateSteps = 1
  randomSeed = 399
  reactants = [electronsGreen electronsRed]
  products = [electronsGreen electronsRed]
</RxnProcess>

<RxnProcess elasticGreenGreen>
  kind = collisionProcess
  rxnPhysics = elasticCollide
  numUpdateSteps = 1
  randomSeed = 399
  reactants = [electronsGreen electronsGreen]
  products = [electronsGreen electronsGreen]
</RxnProcess>

<RxnProcess elasticRedRed>
  kind = collisionProcess
  rxnPhysics = elasticCollide
  numUpdateSteps = 1
  randomSeed = 399
  reactants = [electronsRed electronsRed]
  products = [electronsRed electronsRed]
</RxnProcess>

<RxnPhysics elasticCollide>
  kind = generalCollision

  <RxnRate rxnRate>
    kind = constantCrossSection
    crossSection = 1e-10
  </RxnRate>

  <RxnProductGenerator productGenerator>
    kind = isotropicBinaryElastic
    randomSeed = 828
  </RxnProductGenerator>

</RxnPhysics>
```

Thermal expansion

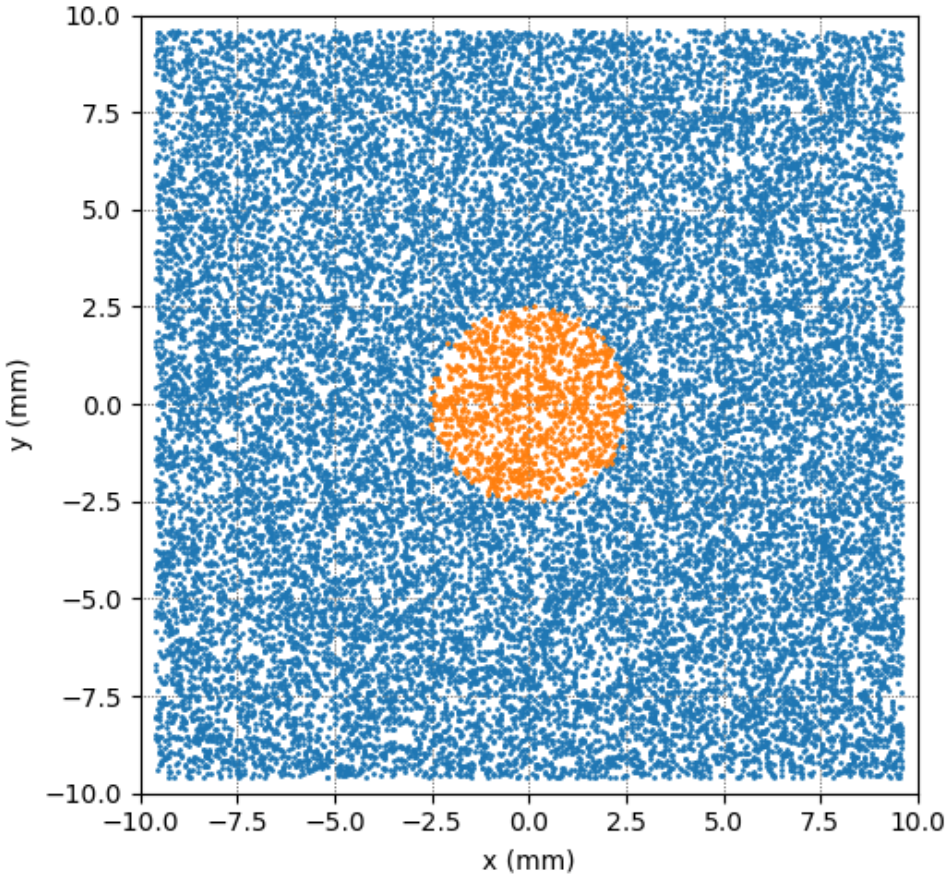
- Two populations of neutral particles (blue and orange)
- Initialized as Maxwellian
  - Orange: $v_{th} = 6 \times 10^5$ m/s
  - Blue: $v_{th} = 6 \times 10^3$ m/s
- Densities equal at $n = 10^{20}$m^3
- Central region expansion limited by collisions with colder plasma
- Binary elastic collisions only

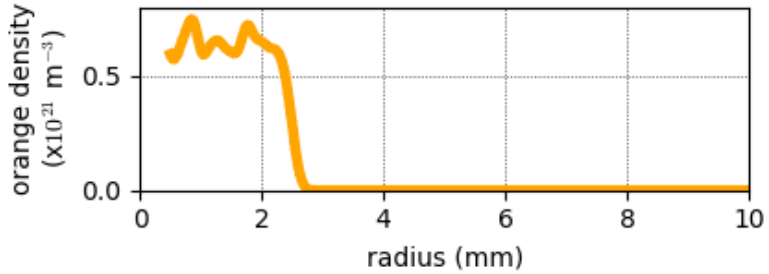


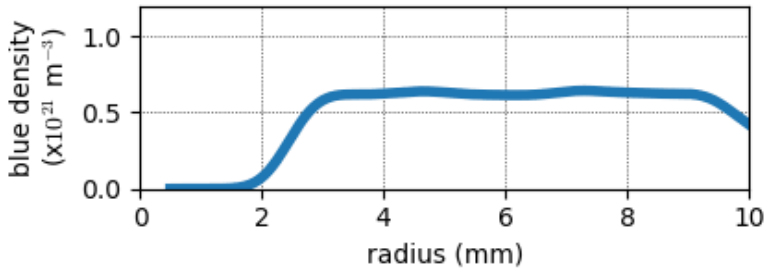
Thermal expansion

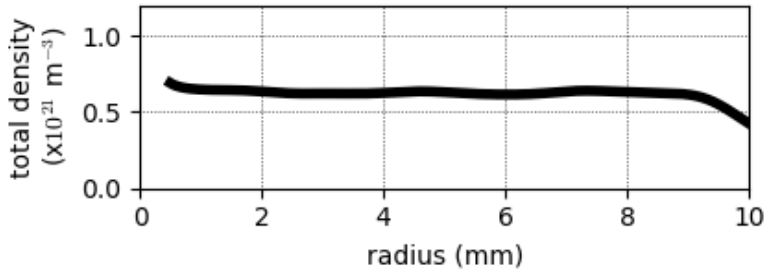


Thermal expansion - no collisions

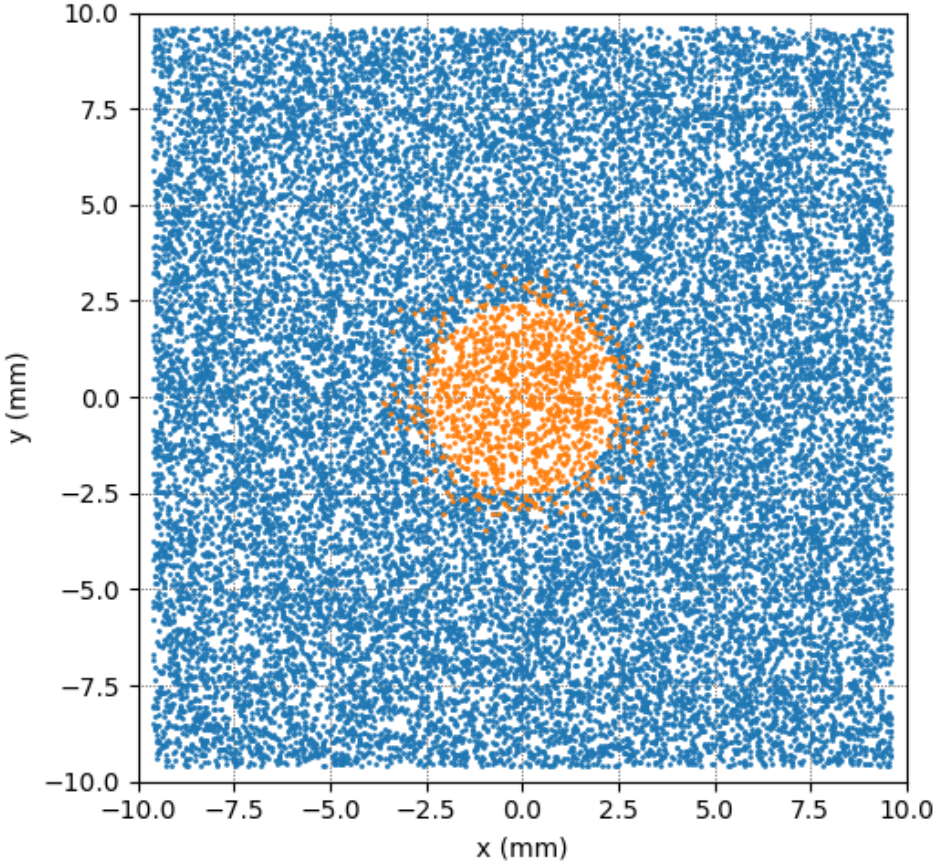


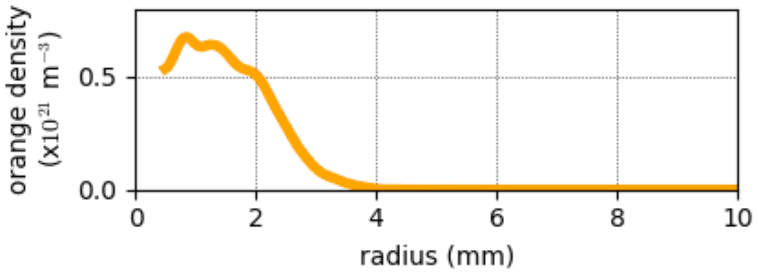


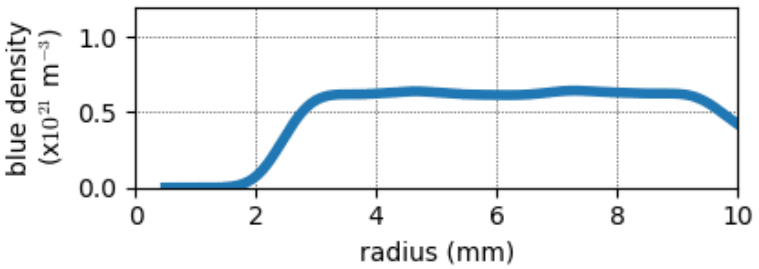


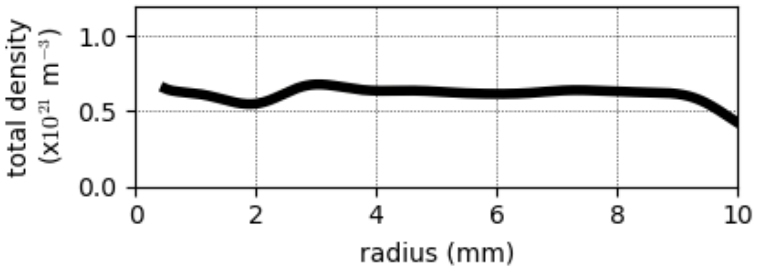


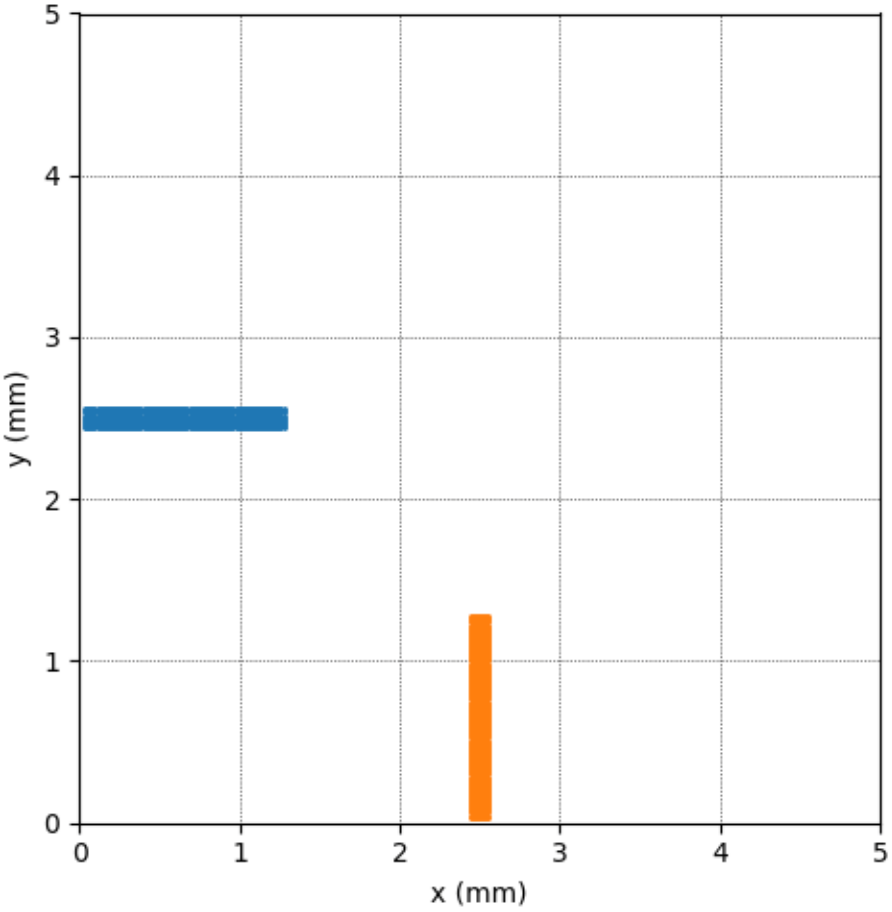
No collisions – bigger dt











Thanks!

Questions?