Smooth Particle Hydrodynamics

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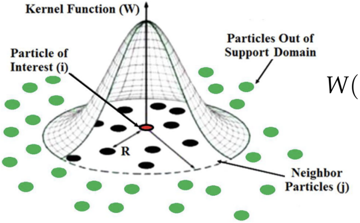
Smoothed Particle Hydrodynamics

- Fluid discretized into particles.
- Physical properties obtained by smoothing over nearby particles using a **kernel**.
- EOM derived from Euler equations



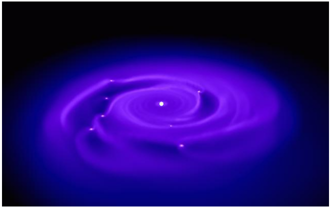
$$W(\mathbf{r}, h) = \sigma(h^d) \begin{cases} \frac{1}{4}(2-q)^3, & 1 \le q \le 2 \\ 1 - \frac{3}{2}q^2(1 - \frac{q}{2}), & 0 \le q \le 1 \\ 0, & q > 1 \end{cases}$$

$$q = \frac{|\mathbf{r}|}{h}$$

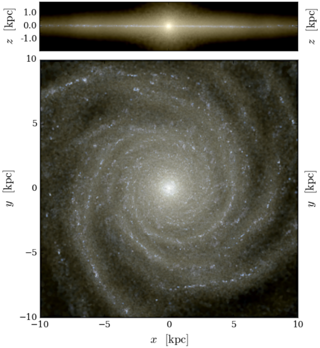
Smoothed Particle Hydrodynamics

- Some examples of SPH:

Gas giant formation simulation (GASOLINE).

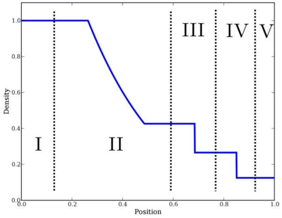


Galaxy modelling (GASOLINE).



Artificial viscosity and entropy

- Addition of a viscosity term to avoid discontinuities from shock waves.
- Entropy is allowed to increase



Example of discontinuity in space in a Shock Tube density profile.

Equations of motion

- Final equations for the particles (with viscosity term):

$$\boxed{\frac{d\mathbf{v}_i}{dt} = -\sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij}\right) \nabla_i W_{ij}(h)}$$

$$\rho_i = \sum_j m_j W(\mathbf{r}_i - \mathbf{r}_j, h), \quad P_i = A_i \rho_i^\gamma$$

$$\frac{dA_i}{dt} = \frac{1}{2} \frac{\gamma - 1}{\rho_i^{\gamma-1}} \sum_{j=1}^{N} m_j \Pi_{ij} \mathbf{v}_{ij} \nabla_i W_{ij}$$

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Approximate Nearest Neighbors

- Put a mesh over the domain
- Put the particles in cells of the mesh
- Use particles from nearby mesh cells for the smoothening

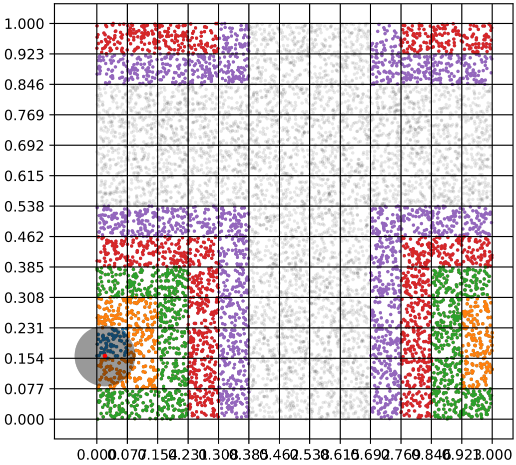

Figure 1: Example nearest-neighbor problem with periodic boundary conditions. The grid corresponds to the mesh used.

The “Hash”

$x_{i,0}$: origin coordinate i

$$\texttt{cell\_idx}(\mathbf{x})_i := \left\lfloor \frac{x_i - x_{i,0}}{\Delta x_i} \right\rfloor \qquad \mathbf{x} \in \mathbb{R}^d.$$

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$$\texttt{cell\_idx}(\mathbf{x})_i := \left\lfloor \frac{x_i - x_{i,0}}{\Delta x_i} \right\rfloor \qquad \mathbf{x} \in \mathbb{R}^d.$$

- How do we store the particles?
- How to retrieve them?

Considering Memory Locality

- IPPL: struct of vectors
- Potential solution: linked lists of indices in each cell

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- IPPL: struct of vectors
- Potential solution: linked lists of indices in each cell
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  $\implies$ sort
- Partition vector by number of particles in each cell
- Copy back in the right order via a temporary

```cpp
template <typename VEC_TYPE, typename D_TYPE>
void sort(const Kokkos::View<VEC_TYPE*>& pos,
          Kokkos::View<D_TYPE*>& target){
    // Current index in each cell
    Kokkos::View<IDX_TYPE*> current_idx("Current Index", ncells);
    Kokkos::deep_copy(current_idx, start_idx);
    // Create temporary
    Kokkos::View<D_TYPE*> temp_target("Temporary", target.size());
    // Copy in the right order
    Kokkos::parallel_for("Reorder-Loop", target.size(),
      KOKKOS_LAMBDA (const IDX_TYPE i){
        const IDX_TYPE key = idx_to_key(cell_idx(pos(i)));
        const IDX_TYPE new_idx =
            Kokkos::atomic_fetch_add(&current_idx(key), 1);
        temp_target(new_idx) = target(i);
      }
    );
    // Copy it back
    Kokkos::deep_copy(target, temp_target);
}
```

Iteration

Iterate over them with a triple loop

```
! Loop over particles
do p_idx = 0, N_particles
    ! Do something with the particle at p_idx
    dummy(p_idx)
    cell_neighbor_idx = get_neighbor_idx(position(p_idx))
    ! Loop over the neighbor cells
    do cell_idx = 0, cell_neighbor_idx.size
        ! Loop over particles in the cell
        do neighbor_idx_offset = 0, cell_size(cell_idx)
            neighbor_idx = start_idx(neighbor_idx(cell_idx))
                         + neighbor_idx_offset
            ! Perform some operation
            do_smth(p_idx, neighbor_idx)
        end do
    end do
end do
```

Iteration

Or even simpler with the help of templates

```
CM.it_over_neighbors(cell_idx, radius,
    [&](const std::size_t i){
        do_smth(i); // i == index of a neighbor
    }
);
```

Scheme choice

- Without viscosity, we choose a leapfrog scheme because it's symplectic.
- With viscosity, there is no Hamiltonian structure, so we choose RK2.

```
Kokkos::parallel_for(N_particles,
  KOKKOS_LAMBDA (const int p_idx){
    x_n(p_idx) = particles.position(p_idx);
    v_n(p_idx) = particles.velocity(p_idx);
    s_n(p_idx) = particles.entropy(p_idx);

    particles.position(p_idx) = x_n(p_idx) + (dt/2)*v_n(p_idx);
    particles.velocity(p_idx) = v_n(p_idx) + (dt/2)*particles.
        accel(p_idx);
    particles.entropy(p_idx) = s_n(p_idx) + (dt/2)*particles.
        d_entropy(p_idx);
    //here expect boundary conditions
}); //need to do a second step !
```

Smoothing kernel size

- For the simplicity we choose to have a constant h. But ideally what we should aim is something like this :

$$h_i^{dim}\rho_i = cste \quad \text{or} \quad h_i^{dim}\rho_i \propto m_i$$

Gridding behavior

- We think that having a constant h leads to this behavior.

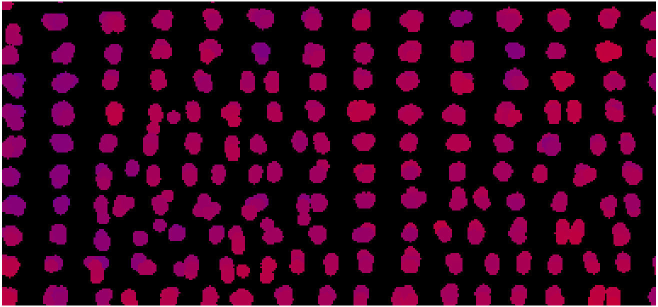

Figure 2: Illustration of the gridding behavior.

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Main codes

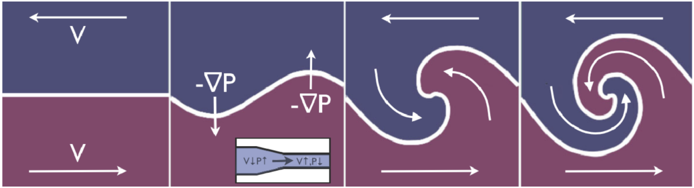
- Declare a Manager object
- Initial particles positions, velocities and entropies
- Integration for certain time domain

```
Manager<1> manager(myparticlelayout, origin, extent, dt, h, 1.4)
    ;
for(unsigned i = 0; i < N_particles; ++i){
    double v = maxwellBoltzmann(T, mass);
    R_part_0.push_back(Vector<double, 1>(origin[0] + extent[0]*i
        /((double)N_particles)));
    v_part_0.push_back(Vector<double, 1>(v));
    m_part_0.push_back(mass);
    entropy_part_0.push_back(1.0);}

//adding initial conditions to the simulation
manager.pre_run(R_part_0, v_part_0, m_part_0, entropy_part_0);
```

Kelvin-Helmholtz Instability

- Fluid flows exerting shear forces on one another
- Interesting behaviour with viscosity
- Instability behaviour at the border between the flows

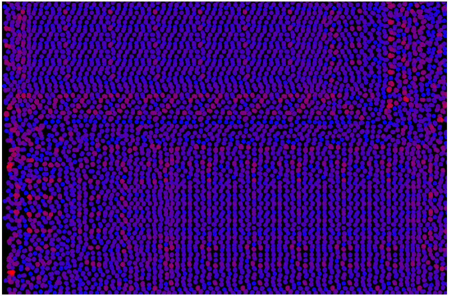


[Gilbert(2017)]

Kelvin-Helmholtz Instability

- Fluid flows exerting shear forces on one another
- Interesting behaviour with viscosity
- Simulation: (preliminary)

$\Longrightarrow$



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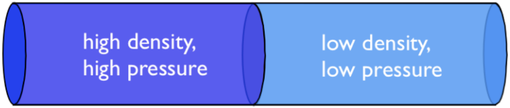
1D Sod-shock tube

- 1D fluid $\rightarrow$ density discontinuity
- Null fluid initial velocity
- Viscous flow $\rightarrow$ shock waves



[Rosswog(2009)]

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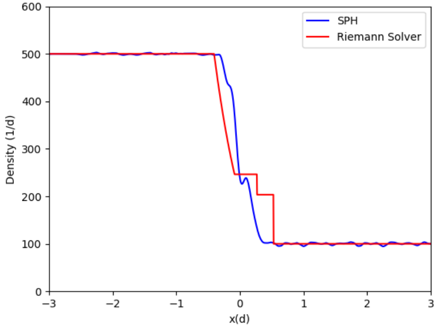

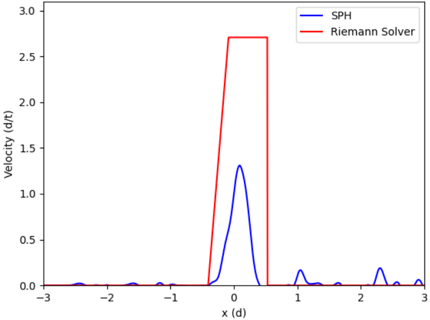

Riemann solver Github

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Conclusions

- Implementation of SPH in C++ using IPPL
- Nearest Neighbor method
- Test cases: KH Instability and shock tube
- "Gridding" Problem
- More work! $\rightarrow$ Adaptive kernel size, add gravity, etc.

Content

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