ColDICE: a parallel Vlasov-Poisson solver using moving adaptive simplicial tessellation

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Sousbie & Colombi, 2016, Journal of Computational Physics, 321, 644

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Code available at github.com/thierry-sousbie/dice

The Vlasov-Poisson equation

Vlasov equation (collisionless)

$$\partial_t f + \mathbf{v} \,.\, \partial_{\mathbf{x}} f - \partial_{\mathbf{x}} \Phi \,.\, \partial_{\mathbf{v}} f = 0,$$

with $f = f\,(t, \mathbf{x}, \mathbf{v})$ the 6D phase space distribution function.

Poisson equation

$$\nabla^2 \Phi = 4\pi G \rho$$
$$\rho = \int f\,(t, \mathbf{x}, \mathbf{v})\, dv,$$

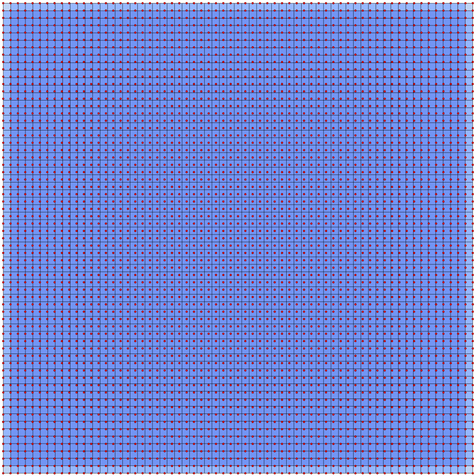
with $\rho = \rho\,(t, \mathbf{x})$ the spatial mass density.

Numerical solution (using macro particles / splitting method)

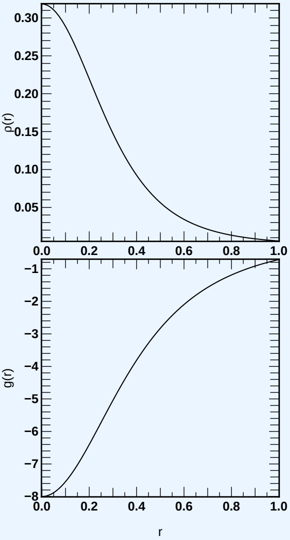
$$\mathbf{x}\,(t + dt/2) = \mathbf{x}\,(t) + \mathbf{v}\,(t)\, dt/2$$
$$\mathbf{v}\,(t + dt) = \mathbf{v}\,(t) - \nabla_{\mathbf{x}} \Phi\,(t + dt/2)\, dt$$
$$\mathbf{x}\,(t + dt) = \mathbf{x}\,(t + dt/2) + \mathbf{v}\,(t + dt)\, dt/2$$

Discreteness effects and Poisson sampling

- Uniform particle distribution
- Static spherically symmetric potential.

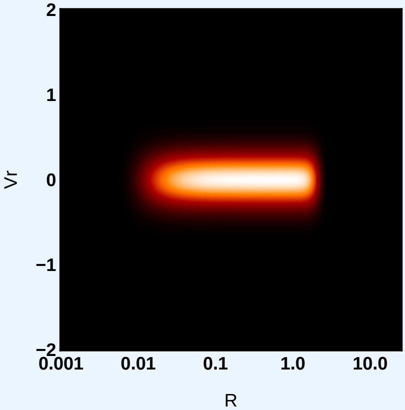


Plummer potential

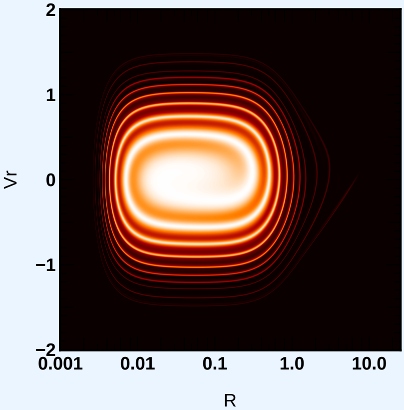


The "cold" approximation (spherically symmetric example)

Phase space PDF $f(0, r, v_r)$

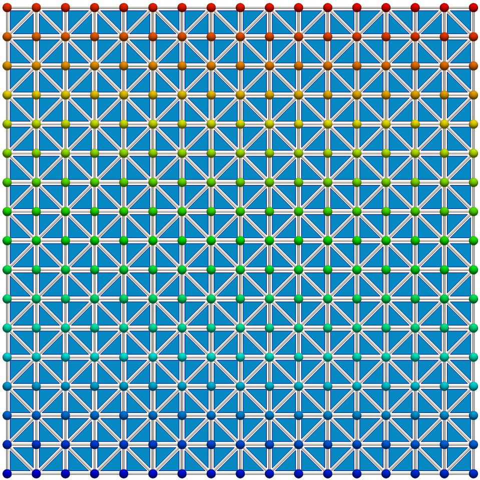


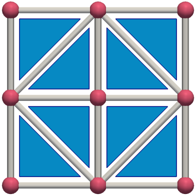
Phase space PDF $f(t, r, v_r)$



- Topology is preserved in phase space
- For "cold" initial conditions, the PDF can be approximated by a "surface" density over a 3D sheet embedded in a 6D phase space.

Phase-space sheet tesselation: 2D

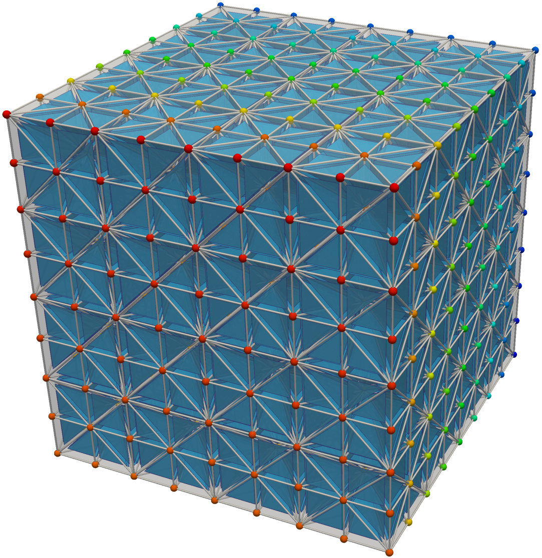


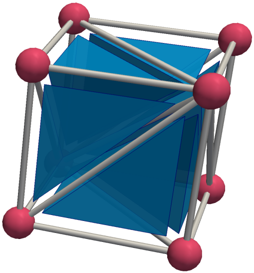


Abel, T., Hahn, O. & Kaehler, R., 2012

Shandarin, S., Habib, S. & Heitmann, K., 2012

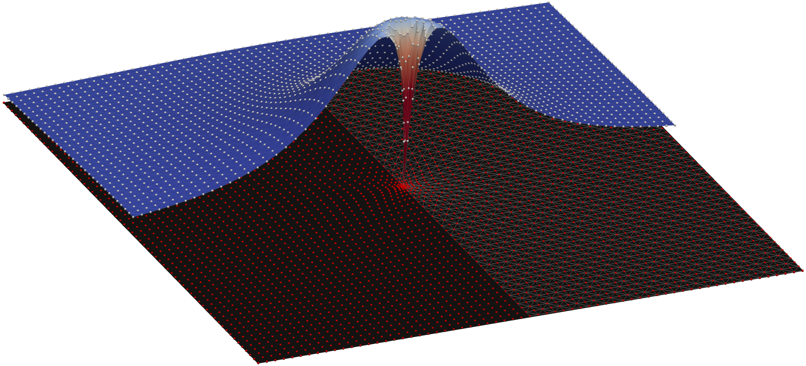
Phase-space sheet tesselation: 3D



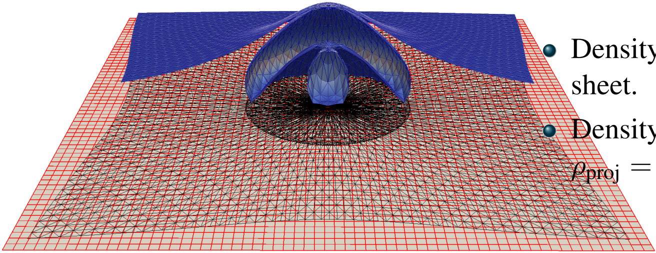


Phase-space sheet evolution in (2+2D) phase space

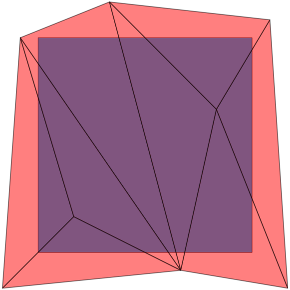
- Static spherically symmetric Plummer potential.
- Phase space sheet represented in $(x, y, \|\mathbf{v}\|)$ space.
- Color proportional to inverse projected volume (i.e. contribution to density)

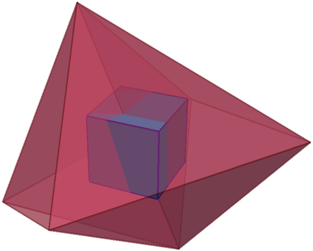


Density sampling from phase-space sheet projection



- Density ρ_{ps} along the sheet.
- Density contribution $\rho_{\mathrm{proj}} = \rho_{\mathrm{ps}}.\mathrm{dV}_{\mathrm{ps}}/\mathrm{dV}_{\mathrm{proj}}$



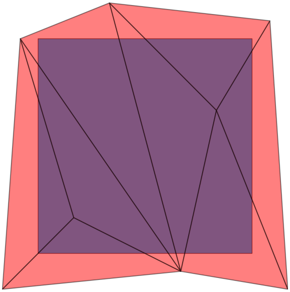


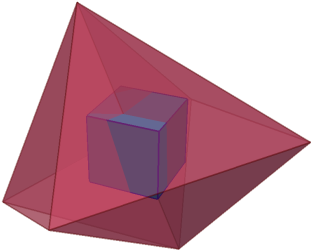
Density sampling from phase-space sheet projection

Exact projected mass in a pixel/voxel

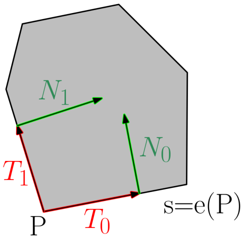
For V a pixel/voxel of a grid:

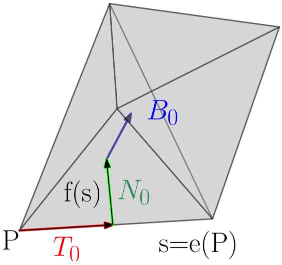
$$M(V) = \sum_i \int_{S_i \cap V} \rho_{\mathrm{proj}}(\mathbf{x})\, d\mathbf{x}$$





A better density estimate: exact projection





$$\mathrm{Vol}_{2D} = \frac{1}{2} \sum_{P} \sum_{e(P)} \mathbf{P}.\mathbf{T}\,\mathbf{P}.\mathbf{N}$$

$$\mathrm{Vol}_{3D} = -\frac{1}{6} \sum_{P} \sum_{s=e(P)} \sum_{f(s)} \mathbf{P}.\mathbf{T}\,\mathbf{P}.\mathbf{N}\,\mathbf{P}.\mathbf{B}$$

Franklin, R. & KankanHalli, M., 1992

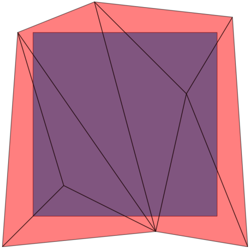
A better density estimate: exact projection

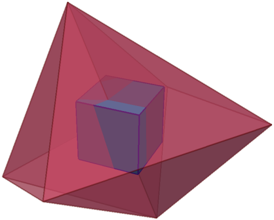
Mass projection

$$M_0\left(V\right) = \sum \rho^0_{\text{proj}} \text{Vol}\left(V \cap S\right) = \sum_{(v,s_v,f_s)\in V} E_0 \rho^0_{\text{proj}}$$

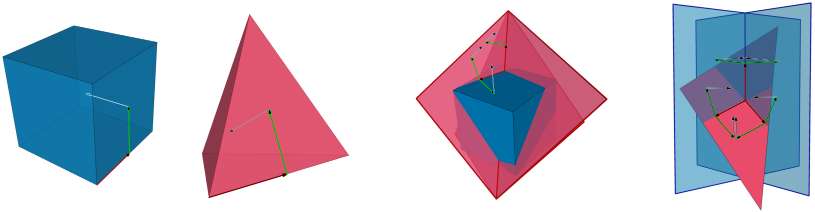
$$M_1\left(V\right) = \sum_{(v,s_v,f_s)\in V} E_0 \left(\rho^0_{\text{proj}} + \mathbf{E_1}.\nabla\rho^1_{\text{proj}}\right)$$

$$\text{with} \begin{cases} E_0^{3D} & = & -\frac{1}{6}\mathbf{P}.\mathbf{T}\,\mathbf{P}.\mathbf{N}\,\mathbf{P}.\mathbf{B}, \\ \mathbf{E_1}^{3D} & = & \frac{1}{4}\left(\mathbf{P}.\mathbf{T}\ \mathbf{T} + 2\mathbf{P}.\mathbf{N}\ \mathbf{N} + 3\mathbf{P}.\mathbf{B}\ \mathbf{B}\right). \end{cases}$$



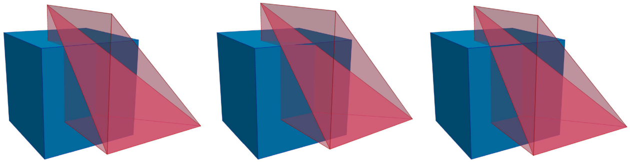


Fast implementation



- For each vertex $[i]$, add all adjacent $(\mathbf{P}, \mathbf{T}, \mathbf{N}, \mathbf{B})$ contributions (2)
- Raytrace edges $[ij]_{i<j}$ through grid, add contributions (3)
- For each face $[ijk]_{i<j,k}$, intersect with grid, add contributions (4)
- For each grid node, add adjacent voxels contributions (1)

Problem: Some configurations are ambiguous at FP precision



Precision and robustness

* **Exact geometric predicates with filtered kernel:** use multi (arbitrary) precison only as required.

$$\mathrm{Or}(\mathbf{p},\mathbf{q},\mathbf{r},\mathbf{s}) = \mathrm{sign}(\mathcal{D}) = \mathrm{sign}\begin{vmatrix} q_x - p_x & q_y - p_y & q_z - p_z \\ r_x - p_x & r_y - p_y & r_z - p_z \\ s_x - p_x & s_y - p_y & s_z - p_z \end{vmatrix},$$

$$E \leq \alpha \prod_{i=1}^{3} \max\left(|q_i - p_i|, |r_i - p_i|, |s_i - p_i|\right).$$

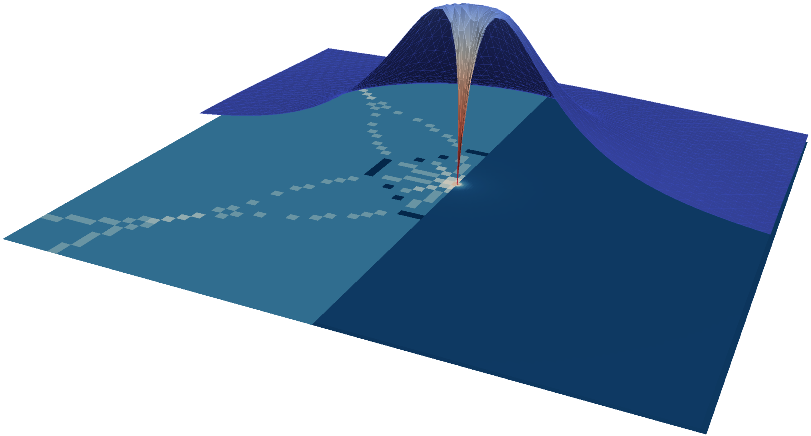
* **Degenerate cases:** Simulation of Simplicity.

$$\mathbf{p} = (p_x, p_y, p_z) \mapsto \mathbf{p}(\epsilon) = (p_x - \epsilon, p_y - \epsilon^2, p_z - \epsilon^3),$$

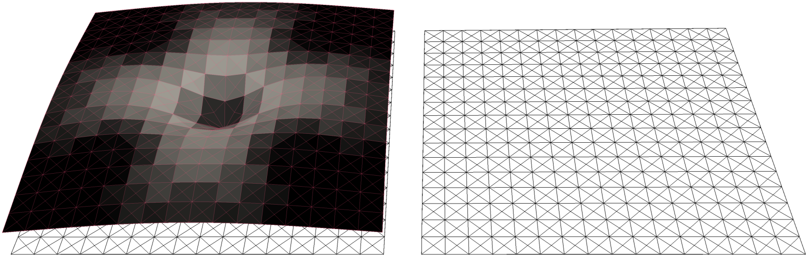
$$\mathcal{D}(\epsilon) = \mathcal{D}(0) + \epsilon \begin{vmatrix} 1 & q_y - p_y & q_z - p_z \\ 1 & r_y - p_y & r_z - p_z \\ 1 & s_y - p_y & s_z - p_z \end{vmatrix} + \epsilon^2 \begin{vmatrix} q_x - p_x & 1 & q_z - p_z \\ r_x - p_x & 1 & r_z - p_z \\ s_x - p_x & 1 & s_z - p_z \end{vmatrix} + \ldots$$

* **Ensure precision of final summation:** Increase dominent terms precision only if required (e.g. large cancelling terms)

A better density estimate: illustration



Tesselation refinement: generic procedure



- Check conserved quantities per simplex (poincaré invariant)
- Refine anisotropically by breaking segments (e.g. the longest)
- Manage refinement conflicts (multipass)
- Try to position the breakpoint close to the sheet in phase space (e.g. second order interpolation of PS sheet)

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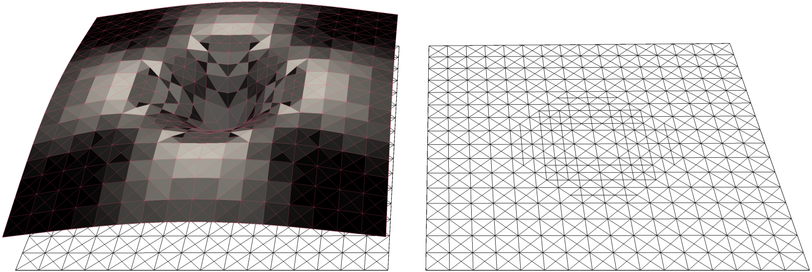

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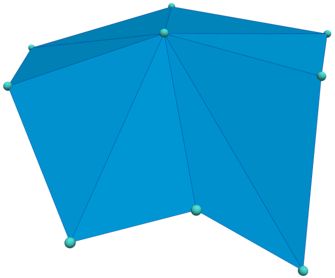
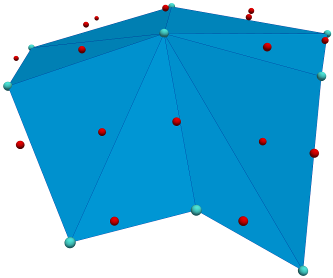
Tesselation refinement



- 1 advected tracer per edge.
- => 2^{nd} order surface.
- Measure worst Poincaré invariants conservation *after* refinement
- Break edges that minimize worst case conservation (multi-pass).
- Advected tracers used as new vertices on refinement.
  $\Rightarrow$ equal mass partitioning.
- New tracers at interpolated lagrangian mid-points over the 2^{nd} order surface.

Tesselation refinement



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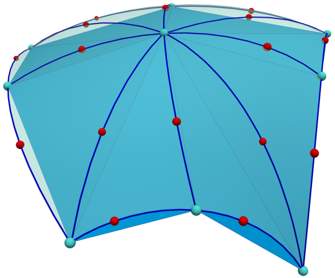

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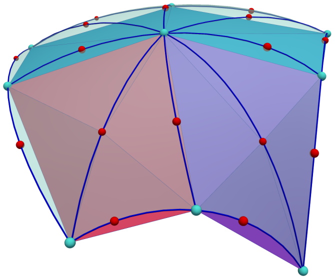

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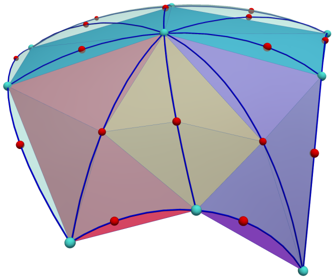

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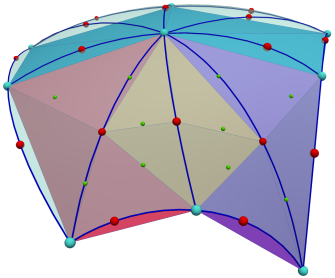

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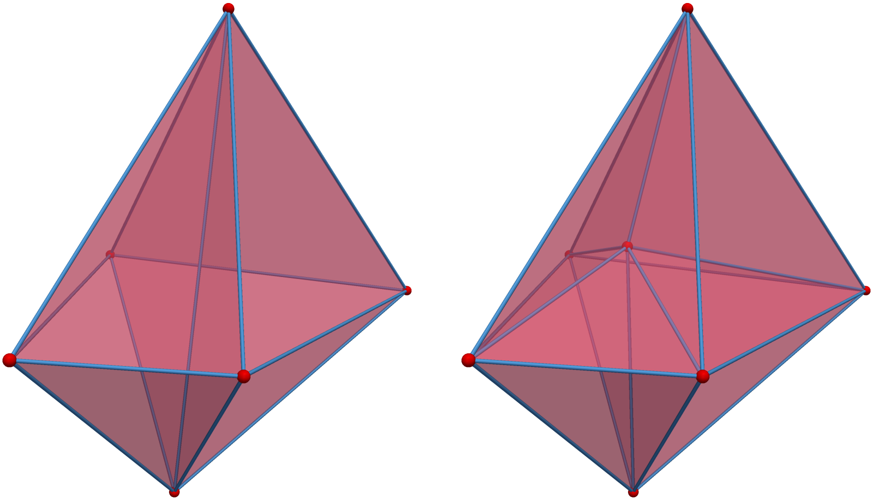
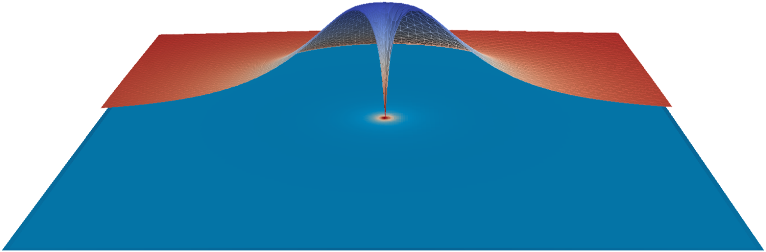
Tesselation refinement (3+3D)



Refining the tesselation: illustration

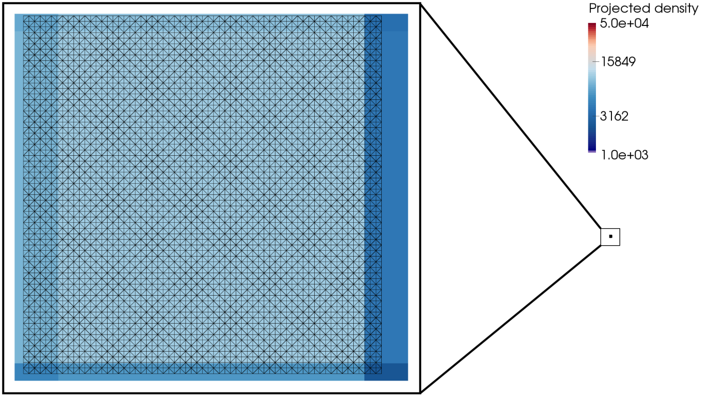


Anisotropic refinement test

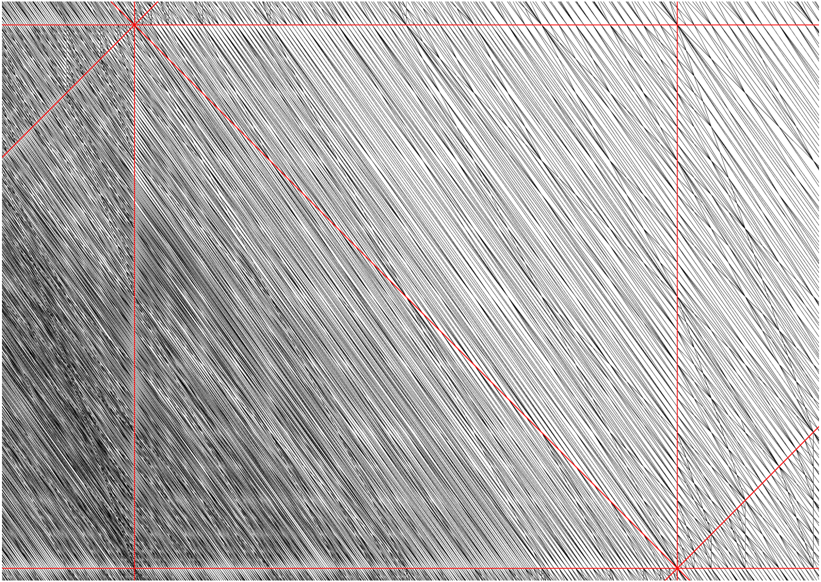
2D static chaotic potential (Binney, 1982)

$$\Phi(x,y) = \frac{1}{2}\log\left({R_c}^2 + x^2 + \frac{y^2}{q^2} - \frac{x^2-y^2}{R_e}\sqrt{x^2+y^2}\right).$$

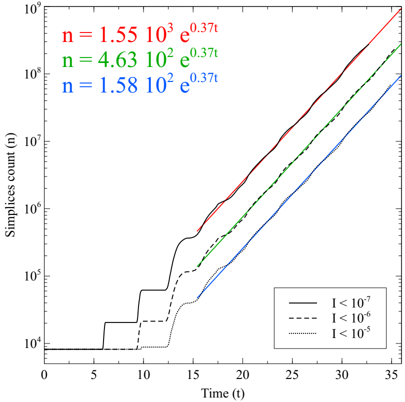
Central radius $R_c = 0.2$, eccentricity $q = 0.9$, chaoticity $R_e = 2$.

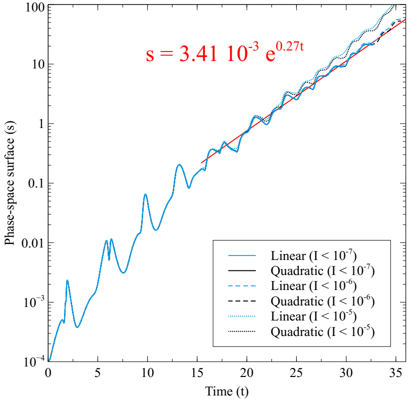


Anisotropic refinement test



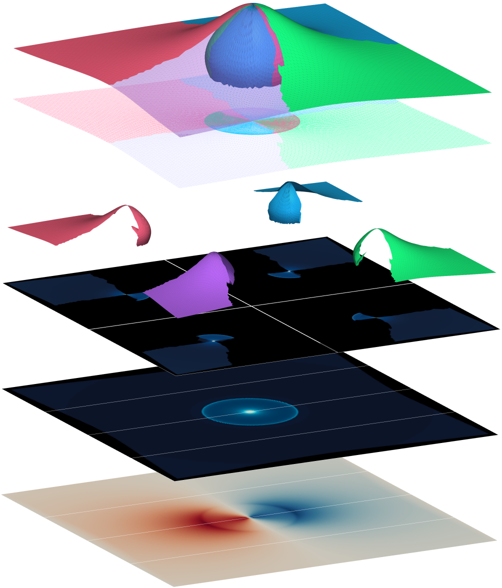
Anisotropic refinement test

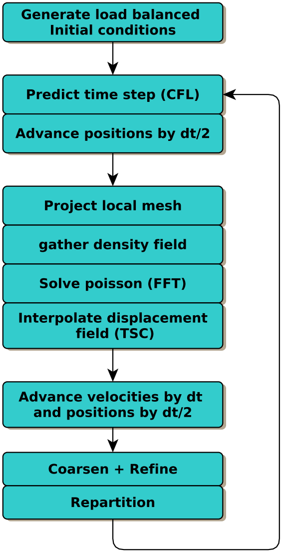




- Theoretical simplices count: $n \propto \epsilon_I^{-\eta_D} (0.46 < \eta_2 < 2/3)$
- Measured simplices count: $n \propto \epsilon_I^{-0.48}$ ($\Rightarrow$ fully anisotropic)
- Phase-space surface: $n \propto s^{3\eta_D} \implies s \propto \exp(0.27t)$

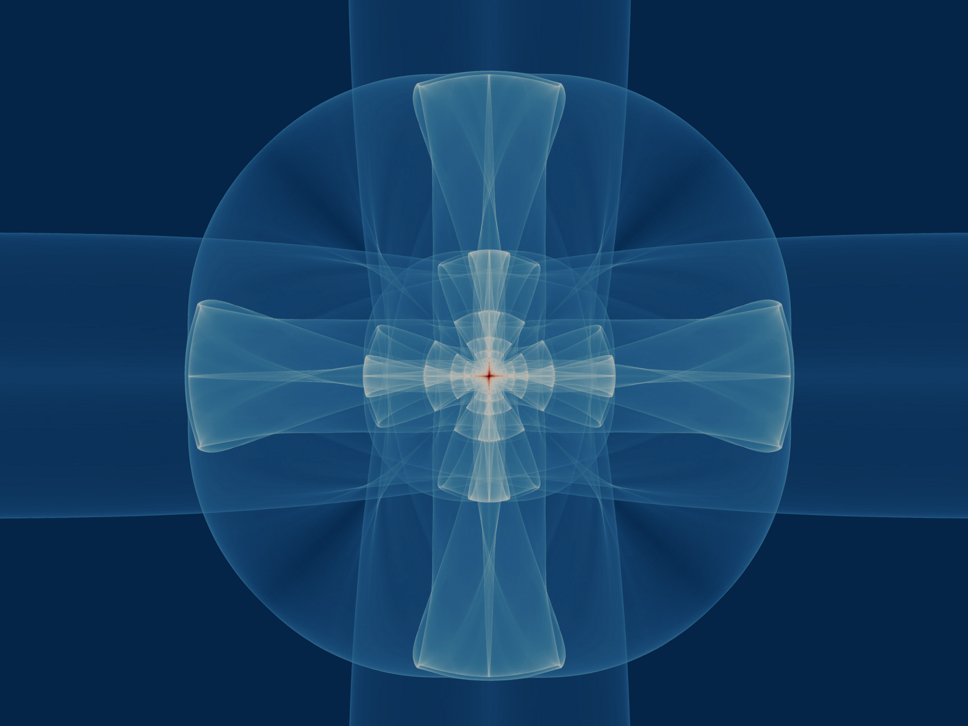
Numerical scheme (openMP + MPI)



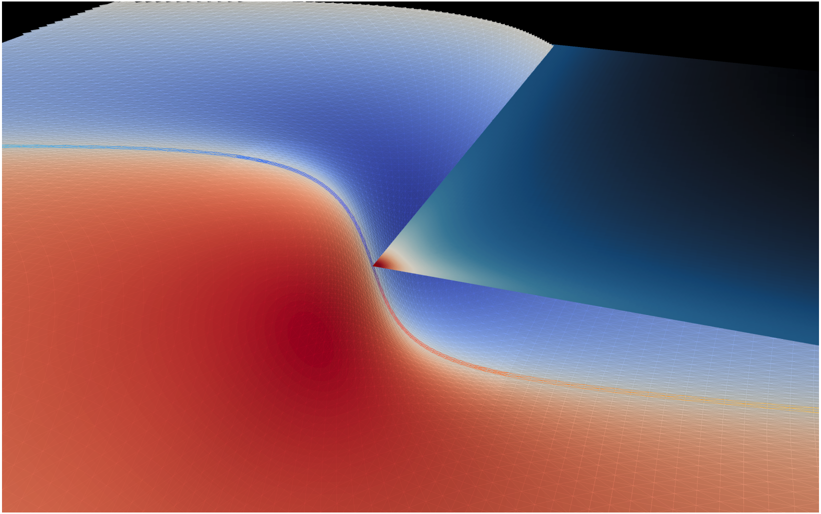


2D sinusoidal waves

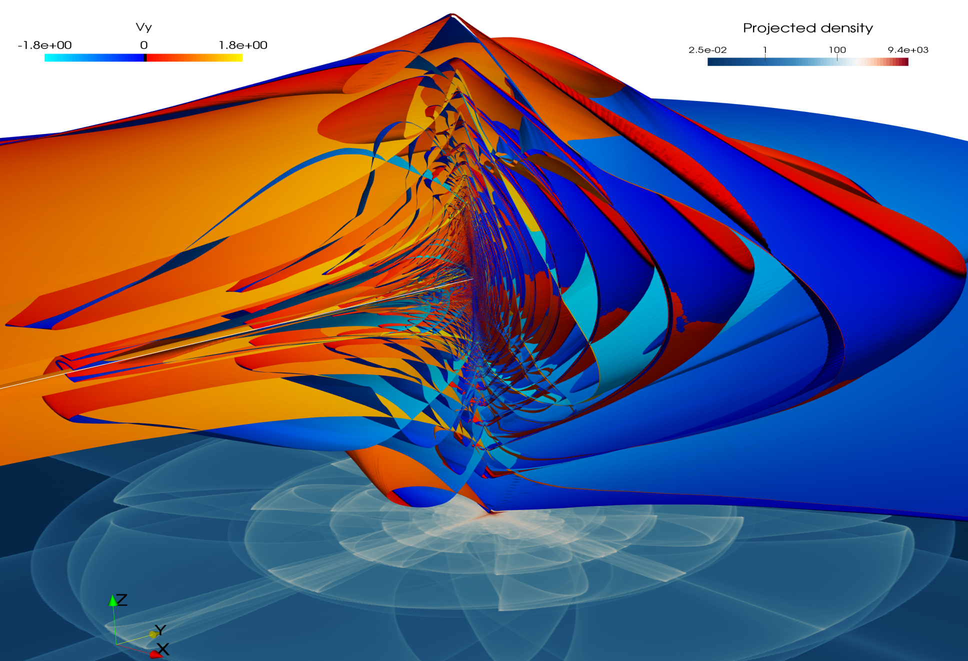
Moutarde & al., 1991, ApJ



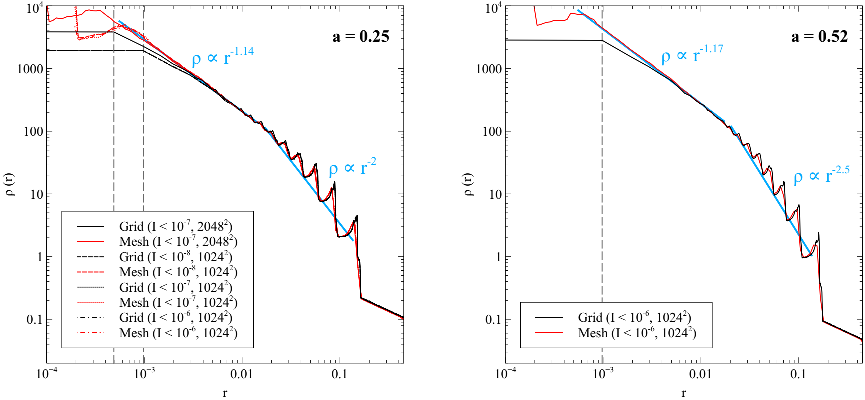
2D sinusoidal waves (phase space evolution)



2D sinusoidal waves (cosmological @$a = 0.25$)

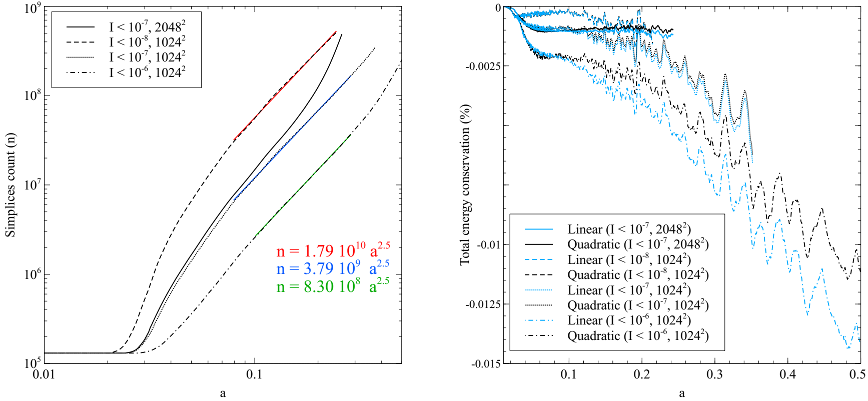


2D sinusoidal waves (cosmological): density profiles



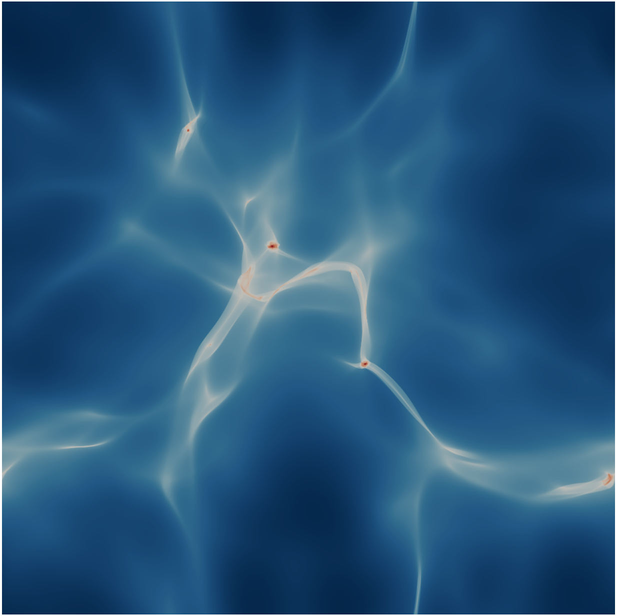
- Density profiles are very consistent between runs.

2D sinusoidal waves (cosmological): energy conservation



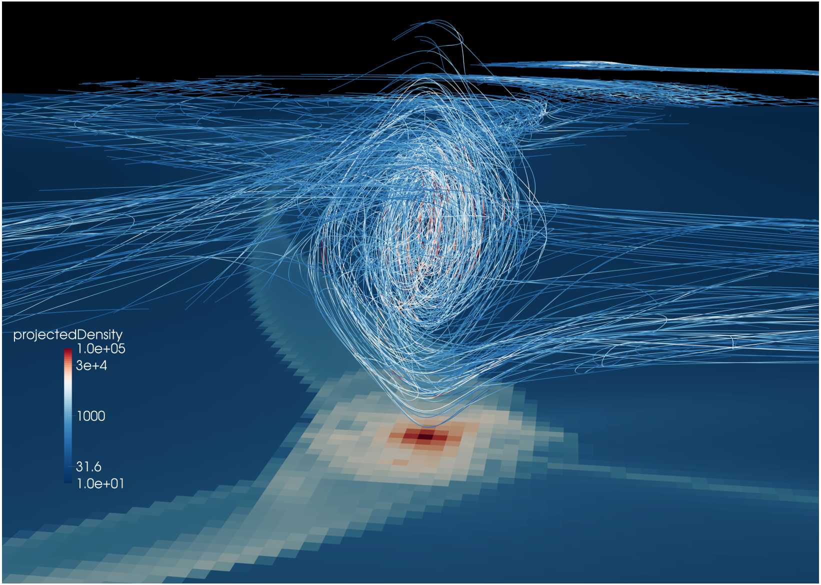
- Refinement is almost isotropic in that case.
- Consistent behavior with ϵ_I ($n \propto a^{2.5}$)
- Very good energy conservation

3D cosmology (WDM)

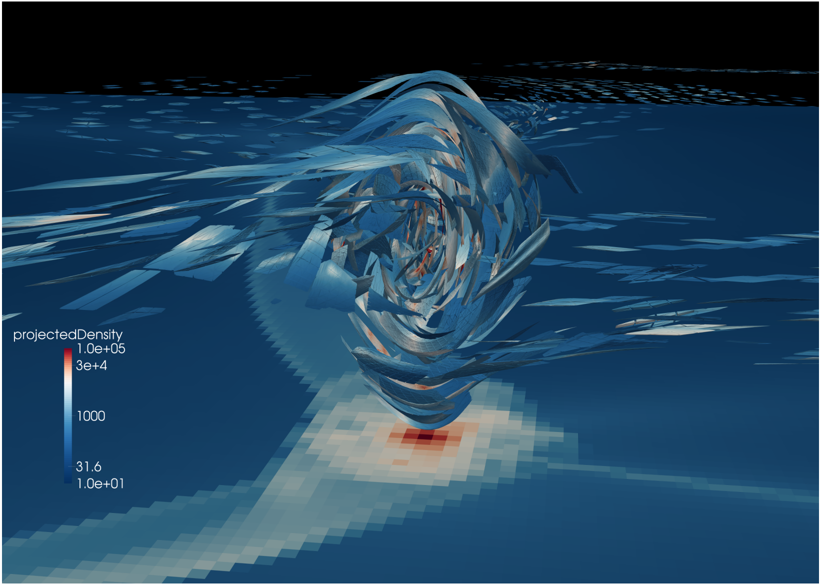


- Warm dark matter
- $M_{\mathrm{WDM}} = 250$ eV
- $L = 20h^{-1}$ Mpc
- $N_G = 1024^3$
- 256^3 init. vertices (+tracers $\Rightarrow 512^3$)
- $\epsilon_I = 10^{-7}$
- $> 10^9$ elements @$a = 0.31$.

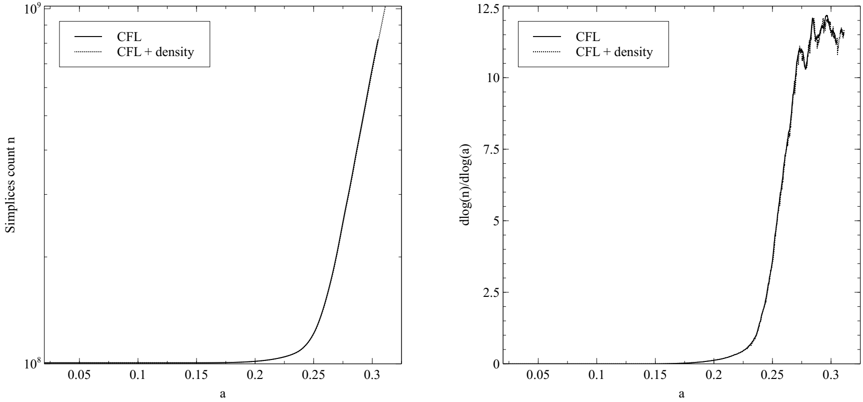
3D cosmology: Lagragian grid (slice)



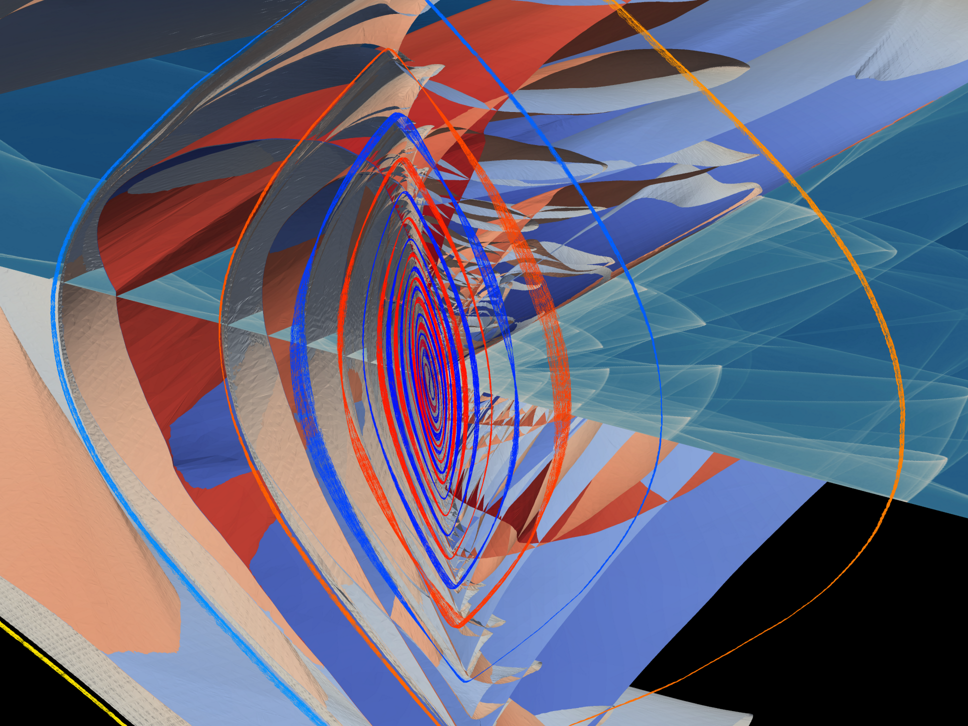
3D cosmology: Lagragian volumes (slice)



3D cosmology: simplices counts



- Very fast growth: $n \propto a^{\alpha}$ with $\alpha \simeq 12 \pm 1/2$
- Need to stop refining at some point to reach $a = 1$ ...



Just for fun ...