## **PiTP Summer School 2009**

### Plan for my lectures

Volker Springel

Lecture 1	Basics of collisionless dynamics and the N-body approach
Lecture 2	Gravitational solvers suitable for collisionless dynamics, parallelization
Lecture 3	More parallelization, Introduction to smoothed particle hydrodynamics
Lecture 4	Algorithmic aspects of SPH, caveats, applications
Lecture 5	Comparison of SPH to finite volume methods, Moving-mesh hydrodynamics





Accuracy issues in cosmological simulations

Different hydrodynamical simulation codes are broadly in agreement, but show substantial scatter and differences in detail THE SANTA BARBARA CLUSTER COMPARISON PROJECT

Frenk, White & 23 co-authors (1999)



#### Mesh codes appear to produce higher entropy in the cores of clusters RADIAL ENTROPY PROFILE Bryan & Norman 1997



10<sup>6</sup>

10<sup>-2</sup>

 $10^{-1}$ 

 $10^{\circ}$ 

r (Mpc)

10<sup>1</sup>

Entropy formulation of SPH also gives somewhat higher core entropy

The entropy profile of the Santa Barbara cluster appears to converge well with SPH, yielding a lower level in the center than found with mesh codes **ENTROPY PROFILES OBTAINED WITH GADGET2 AT DIFFERENT RESOLUTION** 



A cloud moving through ambient gas shows markedly different longterm behavior in SPH and Eulerian mesh codes **DISRUPTION OF A CLOUD BY** 



**Agertz et al. (2007)** 



## Cosmological structure formation is a multi-scale process driven by gravity

AMR codes have difficulty resolving the halo mass function

COMPARISON OF THE DARK MATTER HALO MASS FUNCTIONS IN ENZO AND GADGET

O'Shea et al. (2005)





The codes also show interesting differences in the number of halos as a function of density...



There are principal differences between SPH and Eulerian schemes some FUNDAMENTAL DIFFERENCE BETWEENS SPH AND MESH-HYDRODYNAMICS



## Eulerian

sharp shocks, somewhat less sharp contact discontinuities

(best schemes resolve fluid discontinuities it in one cell)

# mixing happens implicitly at the cell level

(but advection adds numerical diffusivity and may provide a source of spurious entropy)

#### no need for artificial viscosity

(in Godunov schemes)

#### Truncation error not Galilean invariant ("high Mach number problem")

## **self-gravity of the gas done on a mesh** (but dark matter must still be represented by particles)

no explicit conservation of total energy when self-gravity is included

#### Lagrangian



#### shocks broadened over roughly 2-3 smoothing lengths (post-shock properties are correct though)

# mixing entirely suppressed at the particle-level

(no spurious entropy production, but fluid instabilities may be suppressed)

#### requires artificial viscosity

#### **Galilean invariant**

self-gravity of the gas naturally treated with the same accuracy as the dark matter, total energy conserved

## Moving-mesh hydrodynamics with AREPO

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# When the mesh is fixed, the results may change if a bulk velocity is imposed

## KELVIN-HELMHOLTZH INSTABILITY AT 50 x 50 RESOLUTION WITH A FIXED MESH FOR DIFFERENT GALILEI BOOSTS

This was started from a sharp initial contact discontinuity.



Boost both in x- and y- directions

The truncation error in Eulerian codes is not Galilean invariant.

With enough cells, the truncation error can always be reduced, so that for properly resolved initial conditions, effective Galilean invariance is reached.

Nevertheless, this is an unwanted feature that is problematic for simulations of cosmological structure formation. Here the accuracy with which individual galaxies are modeled depends on their velocity magnitude.

## The Riemann problem as basis for high-accuracy Godunov schemes CALCULATION OF THE GODUNOV FLUX



which yields the Godunov flux

## The "upwind side" of the flow depends on the frame of reference THE GODUNOV FLUX IN DIFFERENT REFERENCE FRAMES



 Numerical scheme not Galilean invariant

 $\rho_{\mathsf{F}}(v_{\mathsf{F}}+v)$ 

A moving-mesh Lagrangian finite volume code can combine the advantages of SPH and Eulerian methods KELVIN-HELMHOLTZ INSTABILITY WITH A MOVING MESH CODE

#### AREPO Code

Springel (2008)

$$\rho = 2$$
 $v_x = 0.5$ 
 $P = 2.5$ 

$$\rho = 1$$
  
 $v_x = -0.5$   
 $P = 2.5$ 



50x50 resolution

# Different examples of test problems with the moving-mesh code

High-resolution Kelvin-Helmholtz instability



High-resolution Rayleigh-Taylor instability

#### Sedov-Taylor Exposion



#### Rayleigh-Taylor (with visible mesh)



Voronoi and Delaunay tessellations provide unique partitions of space based on a given sample of mesh-generating points BASIC PROPERTIES OF VORONOI AND DELAUNAY MESHES

#### Voronoi mesh



#### **Delaunay triangulation**



#### both shown together



- Each Voronoi cell contains the **space closest** to its generating point
- The Delaunay triangulation contains only triangles with an **empty circumcircle**. The Delaunay tiangulation maximizes the minimum angle occurring among all triangles.
- The centres of the circumcircles of the Delaunay triangles are the vertices of the Voronoi mesh. In fact, the two tessellations are the topological **dual graph** to each other.

# A finite volume discretization of the Euler equations on a moving mesh can be readily defined

THE EULER EQUATIONS AS HYPERBOLIC SYSTEM OF CONSERVATION LAWS



Equation of state:  $P = (\gamma - 1)\rho u$ 

Discretization in terms of a number of finite volume cells:



But how to compute the fluxes through cell surfaces?

The fluxes are calculated with an exact Riemann solver in the frame of the moving cell boundary **SKETCH OF THE FLUX CALCULATION** 





The velocities of the mesh-generating points uniquely determine the motion of all Voronoi faces

**CHANGE OF VORONOI CELLS AS A FUNCTION OF TIME** 



 $oldsymbol{w} = rac{oldsymbol{v}_{
m R} + oldsymbol{v}_{
m L}}{2} + oldsymbol{w}'$ 

rate of change of volume of a cell

$$\frac{\mathrm{d}V_i}{\mathrm{d}t} = -\sum_{j\neq i} A_{ij} \left[ \frac{\boldsymbol{c}_{ij}}{r_{ij}} (\boldsymbol{v}_j - \boldsymbol{v}_i) + \frac{\boldsymbol{r}_{ij}}{2r_{ij}} (\boldsymbol{v}_j + \boldsymbol{v}_i) \right]$$

$$egin{aligned} m{r}_{ij} &= m{x}_i - m{x}_j \ m{c}_{ij} &= m{f}_{ij} - (m{x}_i + m{x}_j)/2 \end{aligned}$$

(see also Serrano & Espanol 2001)

# To achieve second-order accuracy, we use a **piece-wise linear** reconstruction

**GRADIENT ESTIMATION AND LINEAR RECONSTRUCTION** 



Green-Gauss gradient estimation:

$$\int_{\partial V} \phi \, \mathrm{d}\boldsymbol{n} = \int_{V} \boldsymbol{\nabla} \phi \, \mathrm{d}V.$$

Leads to:

$$\left\langle \boldsymbol{\nabla}\phi\right\rangle_{i} = \frac{1}{V_{i}} \sum_{j\neq i} A_{ij} \left( \left[\phi_{j} - \phi_{i}\right] \frac{\boldsymbol{c}_{ij}}{r_{ij}} - \frac{\phi_{i} + \phi_{j}}{2} \frac{\boldsymbol{r}_{ij}}{r_{ij}} \right]$$

Slope limiting procedure:

$$\left\langle \boldsymbol{\nabla}\phi\right\rangle _{i}^{^{\prime}}=lpha_{i}\left\langle \boldsymbol{\nabla}\phi
ight
angle _{i}$$

$$\alpha_{i} = \min(1, \psi_{ij})$$

$$\psi_{ij} = \begin{cases} (\phi_{i}^{\max} - \phi_{i}) / \Delta \phi_{ij} & \text{for } \Delta \phi_{ij} > 0\\ (\phi_{i}^{\min} - \phi_{i}) / \Delta \phi_{ij} & \text{for } \Delta \phi_{ij} < 0\\ 1 & \text{for } \Delta \phi_{ij} = 0 \end{cases}$$

$$\Delta \phi_{ij} = \langle \nabla \phi \rangle_{i} \cdot (\boldsymbol{f}_{ij} - \boldsymbol{s}_{i})$$

$$\phi_{i}^{\max} = \max(\phi_{j}) \qquad \phi_{i}^{\min} = \max(\phi_{j})$$

Our second-order time integration scheme uses a half-step prediction in primitive variable formulation

#### A MUSCL-LIKE SCHEME



#### And finally...

Update the conserved variables of each cell:  $\boldsymbol{Q}_{i}^{(n+1)} = \boldsymbol{Q}_{i}^{(n)} - \Delta t \sum_{j} A_{ij} \hat{\boldsymbol{F}}_{ij}^{(n+1/2)}$ 

This scheme is **Galilean invariant** if *w* is tied to the fluid velocity. Transform left and right fluid states into rest frame of face

$$oldsymbol{W}_{\mathrm{L,R}}^{\,\prime} = oldsymbol{W}_{\mathrm{L,R}} - \left(egin{array}{c} 0 \ oldsymbol{w} \ 0 \end{array}
ight)$$

Linearly predict the states to the midpoint of the face, and evolve them forward in time by half a timestep:

$$\boldsymbol{W}_{\mathrm{L,R}}^{\prime\prime} = \boldsymbol{W}_{\mathrm{L,R}}^{\prime} + \left. \frac{\partial \boldsymbol{W}}{\partial \boldsymbol{r}} \right|_{\mathrm{L,R}} (\boldsymbol{f} - \boldsymbol{s}_{\mathrm{L,R}}) + \left. \frac{\partial \boldsymbol{W}}{\partial t} \right|_{\mathrm{L,R}} \frac{\Delta t}{2}$$

The prediction in time can be done with the Euler equations:

$$\frac{\partial \boldsymbol{W}}{\partial t} + \boldsymbol{A}(\boldsymbol{W}) \frac{\partial \boldsymbol{W}}{\partial \boldsymbol{r}} = 0 \qquad \boldsymbol{A}(\boldsymbol{W}) = \begin{pmatrix} \boldsymbol{v} & \rho & 0\\ 0 & \boldsymbol{v} & 1/\rho\\ 0 & \gamma P & \boldsymbol{v} \end{pmatrix}$$

Rotate the states such that one coordinate is normal to the face  $\boldsymbol{W}_{\mathrm{L,R}}^{\prime\prime\prime} = \boldsymbol{\Lambda} \, \boldsymbol{W}_{\mathrm{L,R}}^{\prime\prime} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \boldsymbol{\Lambda}_{3\mathrm{D}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \boldsymbol{W}_{\mathrm{L,R}}^{\prime\prime}$ 

Solve the Riemann problem  $\boldsymbol{W} = R_{\text{iemann}}(\boldsymbol{W}_{\text{L}}^{\prime\prime\prime}, \boldsymbol{W}_{R}^{\prime\prime\prime})$ 

Transform the solution back to the calculational frame

$$\boldsymbol{W}_{\mathrm{lab}} = \left( egin{array}{c} \rho \ \boldsymbol{v}_{\mathrm{lab}} \ P \end{array} 
ight) = \Lambda^{-1} \boldsymbol{W} + \left( egin{array}{c} 0 \ \boldsymbol{w} \ 0 \end{array} 
ight)$$

Calculate the net flux in the calculational frame

$$\hat{F} = F(U) - Uw^{\mathrm{T}} = \left(egin{array}{c} 
ho(v_{\mathrm{lab}} - w) \ 
ho v_{\mathrm{lab}}(v_{\mathrm{lab}} - w)^{\mathrm{T}} + P \ 
ho e_{\mathrm{lab}}(v_{\mathrm{lab}} - w) + Pv_{\mathrm{lab}} \end{array}
ight)$$

Eulerian and moving-mesh code are similar in shockcapturing, but differ in the treatment of contact discontinuities

#### COMPARISON OF SOD SOCK TUBES



1.2 Very strong moving mesh 1.0 isothermal rarefaction 2 0.8 waves are better represented by the a 0.6 2 Eulerian approach 0.4 -2 **COMPARISON OF A** 0.2 **STRONG ISOTHERMAL** moving mesh 0.0 **DOUBLE RAREFACTION** -4 -2 2 -4 0 -2 0 2 4 -4 х х 1.2 Eulerian 1.0 0.8 **م** 0.6 2 0 0.4 -2 0.2 Eulerian 0.0 -2 0 2 -2 0 2 -4 4 -4 4 х х 1.2 SPH 1.0 0.8<u>م</u> 0.6 2 0 0.4 -2 0.2 SPH 0.0 -4 -2 0 2 -2 2 4 0 -4 -4 4 х х

#### The moving-mesh code deals well will problems that involve complicated shock interactions woodward & colella's INTERACTING DOUBLE BLAST PROBLEM



#### The Gresho vortex test in two dimensions EVOLUTION OF A STATIONARY VORTEX FLOW

$$\begin{array}{lll} \mbox{Initial} \\ \mbox{conditions:} \end{array} v_{\phi}(r) = \left\{ \begin{array}{ll} 5r & \mbox{for} & 0 \le r < 0.2 \\ 2 - 5r & \mbox{for} & 0.2 \le r < 0.4 \\ 0 & \mbox{for} & r \ge 0.4 \end{array} \right. P(r) = \left\{ \begin{array}{ll} 5 + 25/2r^2 & \mbox{for} & 0 \le r < 0.2 \\ 9 + 25/2r^2 - & \\ 20r + 4\ln(r/0.2) & \mbox{for} & 0.2 \le r < 0.4 \\ 3 + 4\ln 2 & \mbox{for} & r \ge 0.4 \end{array} \right. \end{array} \right.$$





## The Gresho vortex test in two dimensions

#### **EVOLVED AZIMUTHAL VELOCITY PROFILE FOR DIFFERENT CODES AND BOOSTS**



## The Gresho vortex test in two dimensions CONVERGENCE RATE AGAINST ANALYTIC SOLUTION





The "Evrard-Collapse" problem is calculated more ~ accurately by the movingmesh code than by SPH

#### COMPARISON OF SPH WITH A FIXED AND A MOVING MESH

low resolution, equal number of cells/particles



#### Eulerian finite volume codes have problems to accurately conserve total energy in the "Evrard Collapse" problem **EVRARD COLLAPSE WITH FLASH-2.5**

Evrard Collapse



eint switch = 0 - Second Derivative Refinement - 5 levels

Colin McNally (2002, McMaster University)

# The error in the total energy can be substantial in standard treatments to include self-gravity in Eulerian codes

ENERGY ERROR FOR DIFFERENT RESOLUTIONS AND DIFFERENT DISCRETIZATION SCHEMES



# How to construct the Voronoi mesh

# Construction of the Voronoi diagram is most efficiently done by constructing it as dual of the Delaunay tessellation

#### A FEW ALGORITHMS FOR DELAUNAY TRIANGULATIONS

<ul> <li>Divide &amp; Conquer (fastest)</li> </ul>	3D • Sequential insertion
<ul> <li>Sequential insertion</li> </ul>	<ul> <li>Projection of 4D convex hull to 3D</li> </ul>
Sweepline algorithm	Incremental construction
<ul> <li>Projection of 3D convex hull to 3D</li> </ul>	

#### **Sequential insertion:**

- (1) **Point location:** Find triangle/tetrahedron that contains point
- (2) **Point insertion**: Split enclosing triangle/tetrahedron into several simplices
- (3) Flips to restore Delaunayhood: Replace edges/facets around the inserted point if they violate the Delaunay condition (empty circumcircle)

# Most algorithms assume the **general position assumption**

Unfortunately, **degenerate cases** do occur in practice, and induce numerical difficulties due to numerical round-off



How can we consistently break ties?

**1. Step: Locate the triangle that contains the point** 



2. Step: Split the triangle into three triangles

















4. Step: Finished! (Or insert next point)





If the **general position assumption** is not fulfilled, degenerate cases can occur. This makes thinks a lot more complicated. One then needs:

- 1-to-N flips for point insertion when the point lies on an edge
- 2-to-6 flips if the point lies on a face
- 4-to-4 flips for reestablishing Delaunayhood
- Accurate geometric predicates required (difficult! Occasionally requires exact arithmetic)







Degenerate point configurations cause trouble – exact arithmetic is required to guarantee robustness USE OF EXACT ARITHMETIC TO DEAL WITH POINTS IN NON-GENERAL POSITION



Is the point in the left or right triangle?

Or is it exactly on the line?

(boils down to evaluating the sign of geometric tests)

$$T_{\text{InCircle}}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{d}) = \begin{vmatrix} 1 & a_x & a_y & a_x^2 + a_y^2 \\ 1 & b_x & b_y & b_x^2 + b_y^2 \\ 1 & c_x & c_y & c_x^2 + c_y^2 \\ 1 & d_x & d_y & d_x^2 + d_y^2 \end{vmatrix}$$

Delaunay algorithms tend to crash if wrong decisions are made!

We use **exact integer arithmetic** if needed:

• Domain is mapped to floating point numbers in the range [1.0, 2.0]

- Mantissa provides a 53-bit integer with a unique one-to-one mapping to the floating point numbers
- Carry out the geometric test with the GMP-library using long integers

#### Solution

- Calculate maximum round-off error in geometric tests, and check whether result could be incorrect
- If the decision is ambiguous due to floating point round-off, use exact arithmetic instead

The Voronoi mesh of 625 randomly distributed points



## A regularized Voronoi mesh

We would like to have such a mesh:

- Optimal use of available resolution
- No small timesteps • due to accidentally small cell dimensions
- Higher accuracy of spatial reconstruction



Lloyd's algorithm is a simple iterative scheme to create a centroidal Voronoi tessellation MAKING ROUND VORONOI CELLS

Lloyd's algorithm:

- (1) Reposition each mesh-generating point of a Voronoi tessellation to the center-of-mass of its associated cell.
- (2) Reconstruct the tessellation, and repeat step (1).

Converges slowly to centroidal Voronoi tessellation.













# Mesh relaxation would also be very useful for creating quiet initial conditions

AN EXPONENTIAL DISK INITIALIZED WITH A POISSOIN DISTRIBUTION



# How should we shift the points to obtain the desired mesh properties?

#### MAKING OR PRESERVING A "NICE" MESH

Current distribution of points $n(\boldsymbol{x})$ Ideal (desired) distribution of points $n_0(\boldsymbol{x})$ 

Lets assume the displacement field from the current coordinate can be described by:

$$oldsymbol{x}_i = oldsymbol{q}_i + \epsilon \,oldsymbol{d}_i \qquad oldsymbol{d} = -oldsymbol{
abla} \Psi$$

Then to linear order:

$$oldsymbol{v}_i = \mathrm{d}oldsymbol{x}_i/\mathrm{d}oldsymbol{\epsilon} = oldsymbol{d}_i \qquad n_\epsilon(oldsymbol{x} + \epsilonoldsymbol{d}) = \epsilon \; n(oldsymbol{x} + oldsymbol{d}) + (1 - \epsilon) \; n_0(oldsymbol{x}) \qquad rac{\mathrm{d}n}{\mathrm{d}\epsilon} + noldsymbol{
abla} \cdot oldsymbol{v} = 0$$

Yields Poisson equation for displacement:

$$abla^2 \Psi = rac{n(\boldsymbol{x} + \boldsymbol{d})}{n_0(\boldsymbol{x})} - 1 \simeq rac{n(\boldsymbol{x})}{n_0(\boldsymbol{x})} - 1$$

How to set the desired distribution of points?

$$A_{i} \equiv \frac{m_{i}}{\tilde{m}} + \frac{V_{i}}{\tilde{V}} \qquad A_{i} = \tilde{A} \qquad \longrightarrow \qquad n_{0}(\boldsymbol{x}) = \frac{1}{\tilde{A}} \left( \frac{\rho(\boldsymbol{x})}{\tilde{m}} + \frac{1}{\tilde{V}} \right)$$

At the end we have: 
$$\nabla^2 \Psi = \frac{\tilde{A} n(\boldsymbol{x})}{\rho(\boldsymbol{x})/\tilde{m} + 1/\tilde{V}} - 1 \qquad \tilde{A} = \frac{V_{\rm tot}}{\sum_i \left(\rho_i/\tilde{m} + 1/\tilde{V}\right)^{-1}}$$

## An example...



# Our technique for mesh relaxation readily creates good initial conditions for arbitrary initial density fields

**REGULARIZED INITIAL CONDITIONS FOR A POISSON REALIZATION OF AN EXPONENTIAL DISK** 



# A differentially rotating gaseous disk with strong shear can be simulated well with the moving mesh code

MODEL FOR A CENTRIFUGALLY SUPPORTED, THIN DISK

 $\Sigma(r) = \Sigma_0 \exp(-r/h)$ 

$$v_c^2(r) \equiv r \frac{\partial \Phi}{\partial r} = 2 \frac{Gm}{h} y^2 \left[ I_0(y) K_0(y) - I_1(y) K_1(y) \right]$$



The moving-mesh approach can also be used to realize arbitrarily shaped, moving boundaries STIRRING A COFFEE MUG









The Santa Barbara cluster develops a high entropy core with the moving mesh scheme, but this is affected by heating from N-body noise **ENTROPY PROFILE IN THE SANTA BARBARA CLUSTER FOR AREPO AND GADGET** 



## Conclusions

#### I described the novel quasi-Lagrangian hydrodynamical code AREPO. It has the following important features:

- Allows Galilean invariant solutions.
- No artificial viscosity, very low numerical diffusivity, and residual diffusivity is invariant in the presence of bulk flows, well behaved for supersonic flows.
- Automatic Lagrangian adaptivity of the mesh. Conveniently gives near ideal resolution improvements in regions that collapse
- Mesh geometry is very flexible, adjusts resolution to primary flow properties, no preferred directions along coordinate axes
- Code parallelized for distributed memory systems both in 2D and 3D, gravity adopted from Gadget-3 code.
- The code can also be used for fixed meshes, both of Cartesian and unstructured type.
- Moving and curved boundary conditions can be implemented comparatively easily.