Making Sense of the Universe with Supercomputers

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• Adaptive Mesh Refinement in Cosmology: First Stars
• Adaptive Ray-Tracing for Radiation Transport
• The Phase Space Sheet for collision-less fluids
• Outlook

• mostly in collaboration with Greg Bryan, John Wise, Mike Norman, Oliver Hahn, Raul Angulo, Ralf Kähler, Devon Powell
400,000 years after the big bang
Universe at 400,000 years

• Temperature 3000K, fluctuations 1 part in 100,000

• Density 300 per cm$^3$, fluctuations 1 part in 1,000

• Hydrogen 76% & Helium 24%. Ion fraction: 2 part in 100,000

• Dark Matter about 6 times more than baryons

• No observations between 400,000 and 900 million years of the universe! So called Dark Ages.
First Things in the Universe

Physics problem:

- Initial Conditions measured
- Constituents, Density Fluctuations, Thermal History
- Physics: Gravity: DM & Gas, HD, Chemistry, Radiative Cooling, Radiation Transport, Cosmic Rays, Dust drift & cooling, Supernovae, Stellar evolution, etc.

Transition from Linear to Non-Linear:

- Using patched based structured adaptive (space & time) mesh refinement
- Use a computer!

\[
\frac{R_\odot}{R_{\text{Milky Way}}} \approx 10^{-12}
\]

\[
\frac{P_\odot,\text{Kepler}}{t_{\text{Hubble}}(z = 30)} \approx 10^{-12}
\]
Adaptive Mesh Refinement


- Gravity, DM, Gas, Chemistry, Radiation, star formation & feedback, MHD, Cosmic Rays

- > 300,000 lines of code in C++ and F77

- Cosmological Radiation Hydrodynamics adapting in space and time

- Dynamic range up to $10^{15}$ using up to 128 bit precision coordinates in space and time

- Has been run with up to millions of grid patches

- Dynamically load balanced parallel with MPI

- [www.enzo-project.org](http://www.enzo-project.org)
### Primordial Gas Chemistry

<table>
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<tr>
<th>Reaction</th>
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<tbody>
<tr>
<td>(1) ( H + e^- \rightarrow H^+ + 2e^- )</td>
<td>(10) ( H_2^+ + H \rightarrow H_2 + H^+ )</td>
<td>(2) ( H^+ + e^- \rightarrow H + h\nu )</td>
<td>(11) ( H_2 + H^+ \rightarrow H_2^+ + H )</td>
<td>(3) ( He^+ + e^- \rightarrow He^+ + 2e^- )</td>
<td>(12) ( H_2 + e^- \rightarrow 2H + e^- )</td>
<td>(4) ( He^+ + e^- \rightarrow He + h\nu )</td>
<td>(13) ( H_2 + H \rightarrow 3H )</td>
<td>(5) ( He^+ + e^- \rightarrow He^{++} + 2e^- )</td>
</tr>
<tr>
<td>(6) ( He^{++} + e^- \rightarrow He^+ + h\nu )</td>
<td>(15) ( H^- + H \rightarrow 2H + e^- )</td>
<td>(7) ( H + e^- \rightarrow H^- + h\nu )</td>
<td>(16) ( H^- + H^+ \rightarrow 2H )</td>
<td>(8) ( H + H^- \rightarrow H_2 + e^- )</td>
<td>(17) ( H^- + H^+ \rightarrow H_2^+ + e^- )</td>
<td>(9) ( H + H^+ \rightarrow H_2^+ + h\nu )</td>
<td>(18) ( H_2^+ + e^- \rightarrow 2H )</td>
<td>(10) ( H_2^+ + H \rightarrow H_2 + H^+ )</td>
</tr>
</tbody>
</table>

- Reaction 8 is much faster than reaction 7.
- I.e. (7) will continue as long as free electrons are available -> H2 formation timescale = recombination timescale
- However, \( k_7 \propto T^{0.88} \) hence adiabatic contraction important. Requires sufficiently high virial temperatures and so introduces a temperature (mass) scale based on chemistry

\[
T_{vir}^{Chem} \approx 10^3 \text{ K}
\]
Making a proto-star

Simulation: Tom Abel (KIPAC/Stanford), Greg Bryan (Columbia), Mike Norman (UCSD)
Viz: Ralf Kähler (AEI, ZIB, KIPAC), Bob Patterson, Stuart Levy, Donna Cox (NCSA), Tom Abel
© “The Unfolding Universe” Discovery Channel 2002
Zoom in

Note disks within disks which happens routinely in turbulent collapses!

Dynamic range \( \sim 1 \times 10^{12} \).

> 30 levels of refinement
tens of thousands of grid patches
dynamically load balanced
MPI. 16 processors enough

Typically 3 solar mass dm particles
> 8 cells per local Jeans Length
non-equilibrium chemistry
RT effects above \( 1 \times 10^{12} \) cm\(^{-3} \)

Turk & Abel 2007
Formation of the very first stars very well suited to ab initio modeling

Can only increase effective Reynolds number with super-computing
Average properties such as mass and temperature profiles converge reasonably well.
Amount of turbulence, vorticity and magnetic field generated less so.
Mass Scales?

Kelvin Helmholtz

time at ZAMS

$10^3 \, M_\odot / \text{yr}$

$10^2 \, M_\odot / \text{yr}$

$5 \times 10^{-3}$

Abel, Bryan & Norman 2002
First Stars are isolated and very massive

- Theoretical uncertainty: 30 - 300 solar mass

Many simulations with three different numerical techniques and a large range of numerical resolutions have converged to this result. Some of these calculations capture 20 orders of magnitude in density!

Non-equilibrium chemistry & cooling, three body H2 formation, chemical heating, H2 line transfer, collision induced emission and its transport, and sufficient resolution to capture chemo-thermal and gravitational instabilities.

Stable results against variations on all so far test dark matter variations, as well as strong soft UV backgrounds.

CALIFORNIA NEBULA, NGC1499
500 pc = 1,500 light years away
30 pc long
Xi Persei, منكب shoulder of Pleiades:
O7.5III
330,000 solar luminosities
~40 solar masses, Teff=3.7e4K
Focus on point sources


Abel, Wise & Bryan 06, MNRAS. Keeps time dependence of transfer equation using photon package concept from Monte Carlo techniques, yet not using any random numbers.

Adaptive ray-tracing of PhotonPackages using HEALPIX pixelization of the sphere. Photon conserving at any resolution.

Parallel using MPI and dynamic load balancing.

\[
\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \frac{\partial I_\nu}{\partial r} = -\kappa I_\nu
\]

Transfer done along adaptive rays

Case B recombination
Early HII regions in 3D

\[ \rho \]

\[ T \]

\[ x_e \]

\[ f_{\text{H}_2} \]

Abel, Wise & Bryan 07 ApJL

O'Shea, Abel, Whalen & Norman 05

Redshift \( \sim 20 \)

\[ \text{1Myr} \quad \text{2.7Myr} \quad \text{8Myr} \]

150pc \quad 3kpc, 1/4 box
Custom GPU based volume renderer for adaptive grids by Ralf, Kähler, Wise & Abel 2006
Wavelength dependent absorption/emission ray tracing volume renderer uses new optimized time-adaptive data format. 1000 times faster than equivalent software implementation on CPU. Proceedings of Volume Graphics 2006
Feedback changes ICs and stellar masses.

• Input on small scales ...

• Formation of early disks more common?

• Caveat: Small numbers of simulations so far

• Mass range: 10-100 in second generation of metal free stars? This second generation may be much more abundant.
Surprising Life

• No three dimensional stellar evolution calculations but much poorly constrained relevant physics
  • Angular momentum transport
  • Mixing from core, mixing into the atmosphere?
  • Stellar winds, as well as episodic mass loss?
  • Magnetic dynamo? Guaranteed seed field of $\sim 4 \times 10^{-10}$ Gauss from recombination.
• Can do:
  • Proto-stars (1st & 2nd generation)
  • HII regions (HeII & HeIII regions)
  • Metal enrichment & potential GRB remnants
  • Beginning of Cosmic Reionization
• Relevant mass range: 1) 30 - 300 solar mass and 2) 10 - 100 solar mass
Cosmological N-body simulations

- Used to make predictions about the distribution of dark matter in the Universe
- Key results
  - Galaxies are arranged in cosmic web of voids/sheets/filaments/halos
  - Universal spherical Dark Matter density profile (NFW) [not understood from analytical arguments]
  - Predicted mass functions of halos and their clustering and velocity statistics
- Primary tool to study observational consequences of LCDM
  - initial conditions: warm vs cold DM, Gaussian vs non-Gaussian
  - sensitivity on global cosmological parameters such as the total matter content and amount of dark energy, etc.
  - Gravitational Lensing signatures
Cosmological N-body simulations

\[ \dot{x} = v(t) \quad \dot{v}_i = - \sum_{i \neq j}^N G m_i m_j \frac{(x_j - x_i)}{|x_j - x_i|^3} \]

- All modern cosmological simulation codes only differ in how they accelerate the computation of the sum over all particles to obtain the net force.

- End result are simply the positions and velocities of all particles.

- Softening of forces (add \( \varepsilon^2 \) in denominator) avoids singularities.

- Limit \( N \) goes to infinity must give correct answer, right?

- Plummer

\[ \dot{v}_i = - \sum_{i \neq j}^N G m_i m_j \frac{(x_j - x_i)}{|x_j - x_i|^2 + \varepsilon^2}^{3/2} \]
**Gravity:**

**Poisson Equation:** \( \nabla^2 \phi = 4 \pi G \rho \)

**Continuum Description**

**Vlasov Equation:** \( \frac{\partial f}{\partial t} + v \nabla f - \nabla \phi \nabla f = 0 \)

For \( N \to \infty \) identical

**N Point Masses:** \( \mathbf{a}_j = -\sum \frac{G m_i}{|\mathbf{x}_i - \mathbf{x}_j|^2 + \epsilon^2} \frac{(\mathbf{x}_i - \mathbf{x}_j)}{|\mathbf{x}_i - \mathbf{x}_j|} \)

**Particle Picture**

Particle "advection": \( \frac{\partial \mathbf{x}_i}{\partial t} = \mathbf{v}_i \) \( ; \) \( \frac{\partial \mathbf{v}_i}{\partial t} = \mathbf{a}_i \)
Dark Matter

Phase Space

$\frac{\partial f}{\partial t} + V \nabla_x f - \nabla \phi \nabla_v f = 0$

Vlasov Equ.

Use Distribution Function

In Phase Space To Describe Evolution: $f(x, v, t)$

Yes. 7 Dimensions...

Oscillation Along One Spatial Dimension
Discretize Dark Matter Distribution: Mass or Volume?

No Gravity

Count particles in random volumes gives average densities

Think mass between particles → Density known everywhere!
Tessellate 3D manifold & track in 6D phase space

- Natural tessellation splits cube into 6 equal sized tetrahedra
- Mass per tetrahedron = \( \frac{1}{6} \) of N-body particle mass

\[
V = \frac{1}{6} \cdot \left( \frac{5}{2} \right)
\]

\[
\Rightarrow l = \frac{m_p}{6V} = \frac{m_p}{\left( \frac{5}{2} \right)}
\]

- Number of edges of the cube
- Think of lattice
- Looping over

The initial Cartesian (Lagrangian/lattice) lattice generates the 6N tetrahedra.
Density information everywhere in space
All microphysical phase space information available

can probe fine-grained phase space structure.
Cosmic Velocity Fields
Exact Overlap Integrals

- any polyhedra intersections without constructing the overlap
- linear and quadratic function defined over polyhedra
- N-th order polynomial over N-dimensional polyhedron (in prep.)
- fundamental building block for many novel algorithms
- 30 times faster than a recursive algorithm
- Computational Geometry - Patent?
- Powell and Abel (2015) JComP

\[
A = \frac{1}{2} \sum_{e,p} (\hat{n}_e \cdot \mathbf{x})(\hat{n}_p \cdot \mathbf{x})
\]

\[
V = -\frac{1}{6} \sum_{f,e,p} (\hat{n}_f \cdot \mathbf{x})(\hat{n}_e \cdot \mathbf{x})(\hat{n}_p \cdot \mathbf{x})
\]
Enormous accuracy gains with higher order interpolation schemes. Shown here in the test case of a cube evolving in a static potential.

Hahn & Angulo 2015, MNRAS
Angulo et al. in prep.
Warm dark matter halo with refinement and higher order elements
Also applicable to Collision-less Plasmas
Example: Landau Damping in 1D

Kates-Harbeck, Totorica, Zrake & Abel 2015, JCompPhys
abs(j_x) with log norm color scale
CIC 16X Resolution

\[ \omega_{pe} t = 25.9 \]
abs(j_x) with log norm color scale
Triangles 16X Resolution

\( \omega_{pe} t = 25.9 \)
Lagrangian Tessellation: What’s it good for?

- Analyzing N-body sims, including web classification, velocity dispersion, profiles, resolution study (Abel, Hahn, Kaehler 2012)
- DM visualization (Kaehler, Hahn, Abel 2012)
- Better Numerical Methods (Hahn, Abel & Kaehler 2013, Hahn, Angulo & Abel 2014-)
- Finally reliable WDM mass functions below the cutoff scale (Angulo, Hahn, Abel 2013)
- Gravitational Lensing predictions (Angulo, Chen, Hilbert & Abel 2014)
- Cosmic Velocity fields (Hahn, Angulo, Abel 2014)
- The SIC method for Plasma simulations (Vlasov/Poisson) (Kates-Harbeck, Totorica, Zrake & Abel 2015, JComp)
- Exact overlap integrals of Polyhedra (Powell & Abel 2015 JComp.)
- Void profiles, Wojtak, Powell, Abel 2016 ArXive : 1602.08541
- your application here ...
Final Remarks

- In Astrophysics very few problems can be addressed in a laboratory setting and computation takes a special case including “discovery” science.

- Many non-linear time-dependent physics applications lead to ever more complex solutions which require ever more memory to be represented.

- Adaptivity is completely essential to these problems. This is true in space, time, phase-space (angles too).

- (Perhaps unsurprisingly) Monte Carlo methods often are neither accurate nor efficient. However, they parallelize well and are much simpler to develop.