

Computational Challenges in Relativistic Cosmology

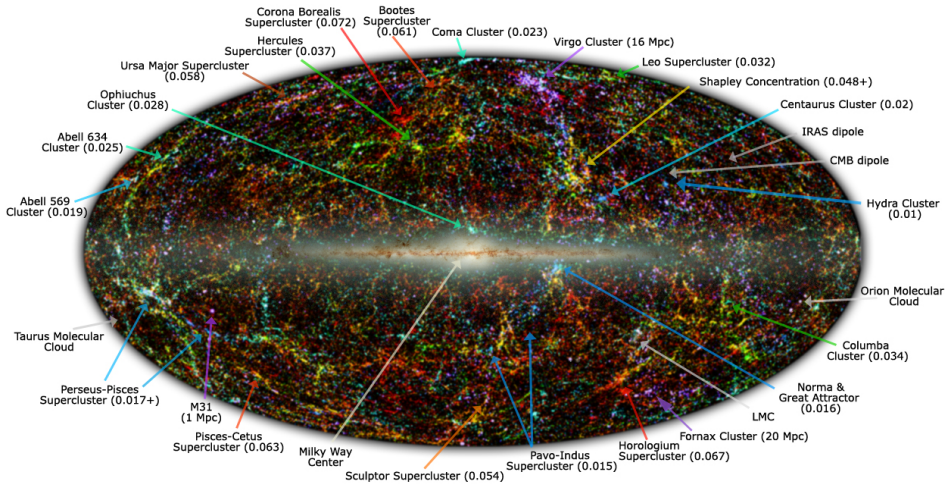
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University of Illinois at Urbana-Champaign (UIUC)

July 4th, 2017

Classical Numerical Cosmology

The local Universe



High performance cosmological simulations

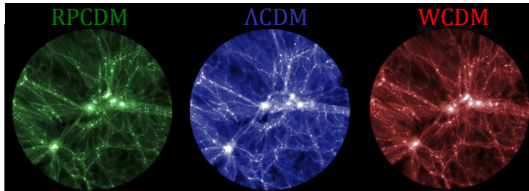
Vlasov-Poisson equations

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\vec{p}}{a^2} \cdot \frac{\partial f}{\partial \vec{x}} - \vec{\nabla} \Phi \cdot \frac{\partial f}{\partial \vec{p}} = 0$$

$$\nabla^2 \Phi = 4\pi G a^2 \bar{\rho} \delta \quad \delta = \frac{\rho - \bar{\rho}}{\bar{\rho}}$$

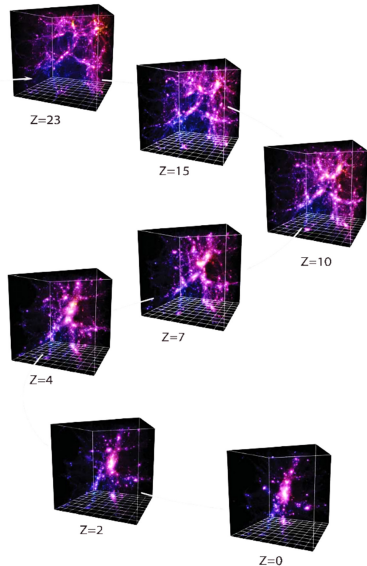
2 regimes

- linear regime $\delta \ll 1$
- non-linear regime $\delta > 1$



Numerical simulation

► **Need of HPC to explore non-linearities**



Distances and perturbations

Homogeneous FLRW metric

$$ds^2 = -c^2 dt^2 + a(t)^2 (dx^2 + dy^2 + dz^2)$$



Perturbed FLRW metric

$$ds^2 = -c^2 \left(1 + 2 \frac{\Phi}{c^2}\right) dt^2 + a(t)^2 \left(1 - 2 \frac{\Phi}{c^2}\right) (dx^2 + dy^2 + dz^2)$$



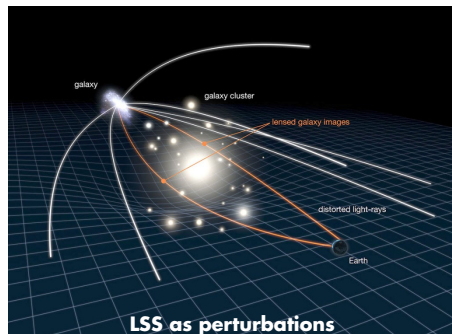
Affine connections

$$\Gamma_{\beta\gamma}^{\alpha} = \frac{1}{2} g^{\alpha\delta} \left(\frac{\partial g_{\delta\beta}}{\partial x^{\alpha}} + \frac{\partial g_{\delta\gamma}}{\partial x^{\beta}} - \frac{\partial g_{\beta\gamma}}{\partial x^{\delta}} \right)$$

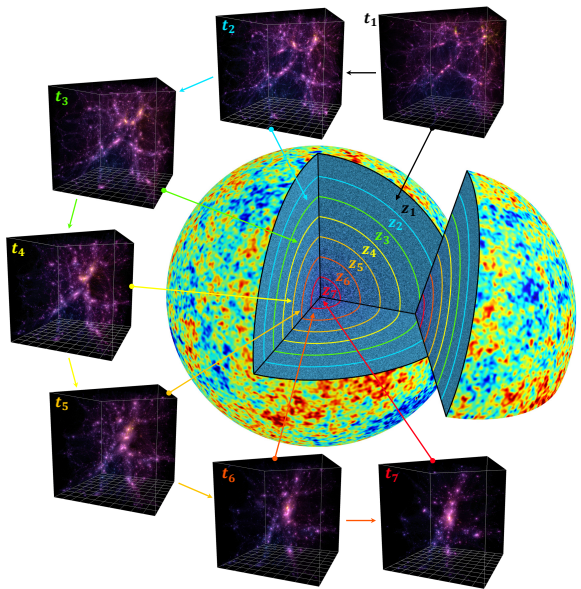


Geodesics equation

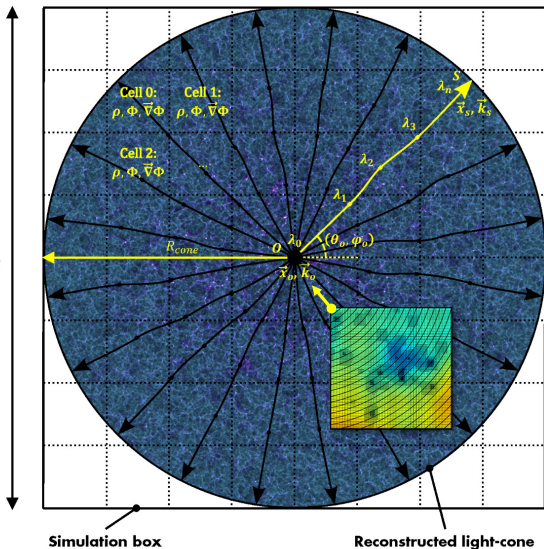
$$\frac{d^2 x^{\alpha}}{d\lambda^2} = -\Gamma_{\beta\gamma}^{\alpha} \frac{dx^{\beta}}{d\lambda} \frac{dx^{\gamma}}{d\lambda}$$



Cone construction



Integration of geodesics



Generic approach

► Direct integration of geodesics

Integration of geodesics

$$\frac{d^2\eta}{d\lambda^2} \approx -\frac{2a'}{a} \frac{d\eta}{d\lambda} \frac{d\eta}{d\lambda} - \frac{2}{c^2} \frac{d\Phi}{d\lambda} \frac{d\eta}{d\lambda} + 2 \frac{\partial\Phi}{\partial\eta} \left(\frac{d\eta}{d\lambda} \right)^2$$

$$\frac{d^2x}{d\lambda^2} \approx -\frac{2a'}{a} \frac{d\eta}{d\lambda} \frac{dx}{d\lambda} + \frac{2}{c^2} \frac{d\Phi}{d\lambda} \frac{dx}{d\lambda} - 2 \frac{\partial\Phi}{\partial x} \left(\frac{d\eta}{d\lambda} \right)^2$$

$$\frac{d^2y}{d\lambda^2} \approx -\frac{2a'}{a} \frac{d\eta}{d\lambda} \frac{dy}{d\lambda} + \frac{2}{c^2} \frac{d\Phi}{d\lambda} \frac{dy}{d\lambda} - 2 \frac{\partial\Phi}{\partial y} \left(\frac{d\eta}{d\lambda} \right)^2$$

$$\frac{d^2z}{d\lambda^2} \approx -\frac{2a'}{a} \frac{d\eta}{d\lambda} \frac{dz}{d\lambda} + \frac{2}{c^2} \frac{d\Phi}{d\lambda} \frac{dz}{d\lambda} - 2 \frac{\partial\Phi}{\partial z} \left(\frac{d\eta}{d\lambda} \right)^2$$

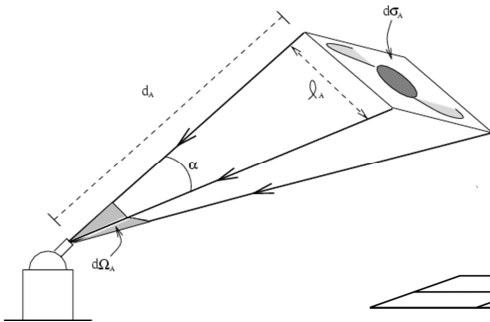
DEUS-FUR + MAGRATHEA

- Full-sky light cones from FUR
- Billions of AMR cells/observer
- 1 million photon/observer
- Minimum number of approx

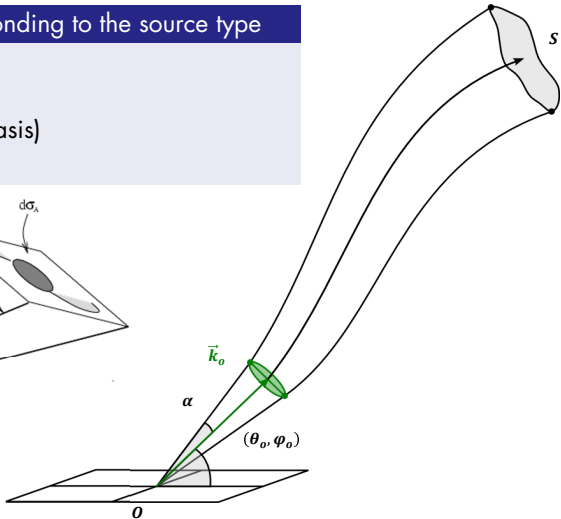
Perturbed trajectories and stop condition

Different possibilities corresponding to the source type

- Affine parameter
- Time
- Perpendicular plane (Sachs basis)
- **Redshift**



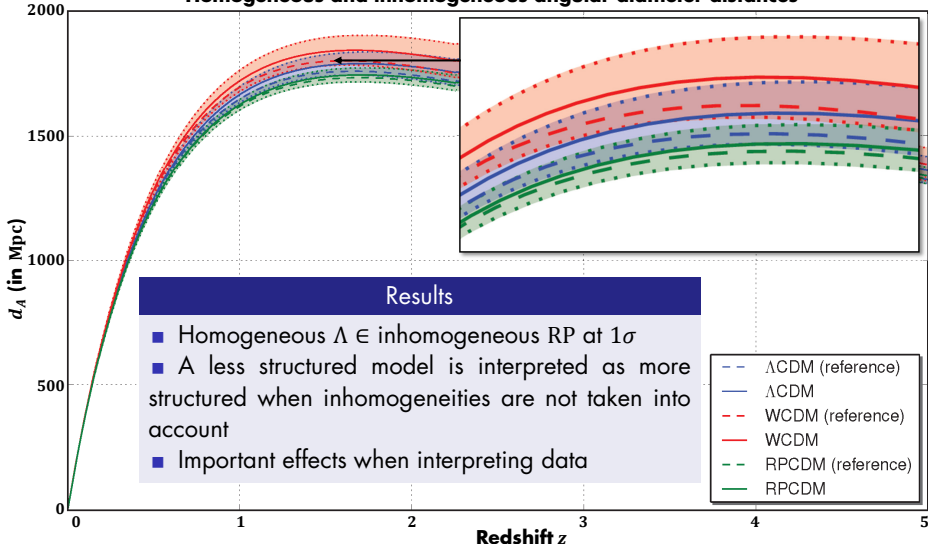
Unperturbed angular diameter distance



Perturbed angular diameter distance

Results

Homogeneous and inhomogeneous angular diameter distances



Defining Numerical Relativistic Cosmology

Where do we want to go? Defining the ideal simulation

Let's imagine we have a yottascale (10^{24}) supercomputer: 1 billion times more powerful than today with 1 billion times more memory than today

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What physics?

- Pure gravity
- Hydrodynamics?
- Baryonic physics?
- Singularities and black holes?
- Neutrinos?
- Magnetic fields?
- Pre-CMB physics?
- etc. . .

Why?

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- Anything else?

Why more power?

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Does not really bring any new knowledge...

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On multiphysics simulations

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- Increased degeneracy
- Add dimensions in a parameter space with local extrema

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- Mimicking reality does not provide any guarantee of correctness
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- Multiphysics increase confusion instead of explainability

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(Personal) conclusion

Simulations are not about the result, they are about the process

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- Understanding emergence

Current Limitations in Numerical Relativistic Cosmology

What do we have? What do we need?

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What we do have

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What we do need

⇒ Therefore it is a problem of computational power

Computational power

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Present and future

- We already have petascale supercomputers (10^{15} FLOPS)
- Exascale supercomputers are coming (10^{18} FLOPS)

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- A lot of time in current simulation codes is spend doing nothing
- Lot of opportunity for optimizations at the bottom of computing
- Computer science, computer architecture, compiler, programming languages

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Applications			
High level libraries			
Wrappers and bindings	Python	R	Java
Optimized libraries	Interpreters (Python, R...)		Virtual machines (JVM)
Compiled, native, low level languages (C, C++...)			
Compilers, mostly written in C and C++ (GCC, LLVM...)			
Machine layer, assembly instructions			

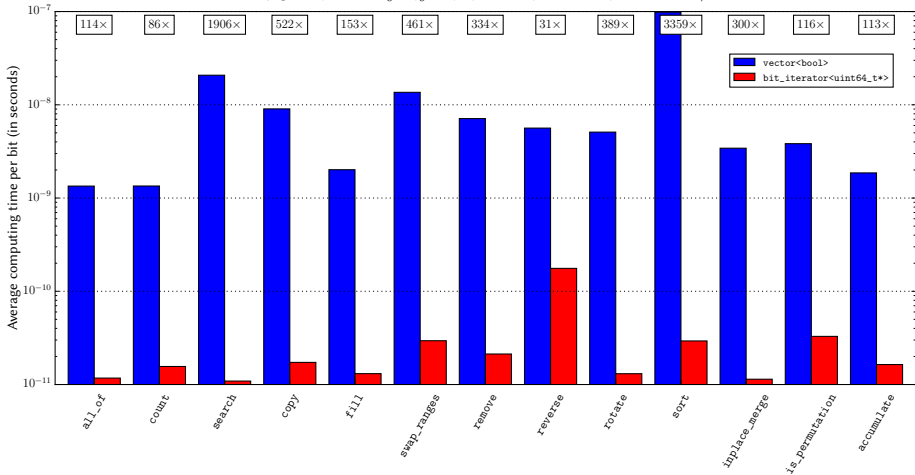
Propagation of optimizations

Softwares are built as stacks. Low-level optimizations can be propagated back to the higher levels while ensuring maximum performances and genericity.

Example of optimization: bit level parallelism

Benchmark of standard algorithms on `vector<bool>` vs their `bit_iterator` specialization (logarithmic scale) [preliminary results]

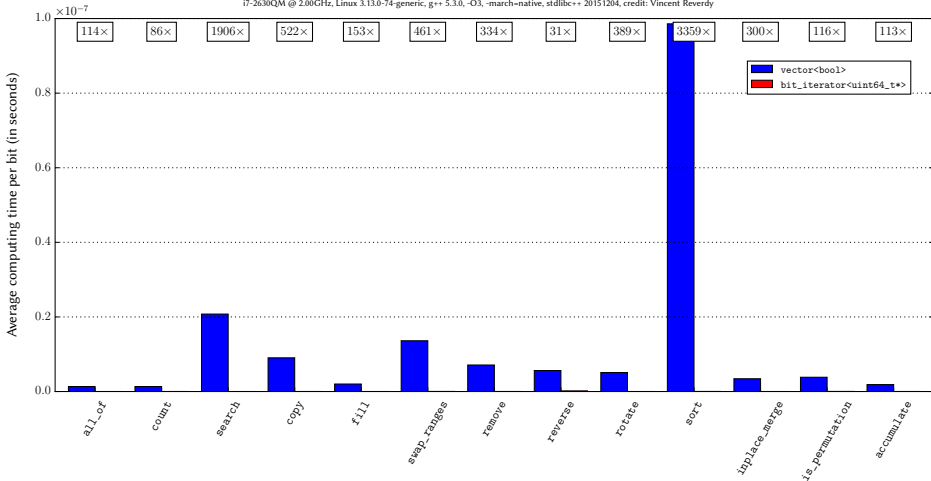
Average time for 100 benchmarks with a vector size of 100,000,000 bits (speedups are provided at the top of each column)
i7-2630QM @ 2.00GHz, Linux 3.13.0-74-generic, g++ 5.3.0, -O3, -march-native, stdlibc++ 20151204, credit: Vincent Reverdý



Bit level parallelism (available in a next revision of C++)

Benchmark of standard algorithms on `vector<bool>` vs their `bit_iterator` specialization (linear scale) [preliminary results]

Average time for 100 benchmarks with a vector size of 100,000,000 bits (speedups are provided at the top of each column)
i7-2630QM @ 2.00GHz, Linux 3.13.0-74-generic, g++ 5.3.0, -O3, -march=native, stdlibc++ 20151204, credit: Vincent Reverdý



Challenges in Numerical Relativistic Cosmology

Upcoming challenge: data structures

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DATA TRANSFER TIMINGS (CREDITS: GOOGLE RESEARCH)		
Operation	Approx. time	Remark
L1 cache reference	0.5 ns	
One cycle on a 3 GHz processor	1 ns	
Branch mispredict	5 ns	
L2 cache reference	7 ns	14× L1 cache
Mutex lock or unlock	25 ns	
Main memory reference	100 ns	200× L1 cache
Send 1 KB over a 1 Gbps network	10 μs	
Read 1 MB sequentially from main memory	250 μs	
Round trip within the same datacenter	500 μs	
Read 1 MB sequentially from a SSD	1 ms	4× memory
Disk seek	10 ms	20× datacenter RT
Read 1 MB sequentially from disk	20 ms	80× memory
Send packet California→Netherlands→California	150 ms	

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Consequences

- Most of the time, pure computing time is not the problem anymore
- Most of the time, data transfer is the problem:
[disk] → [memory] → [cache]
[cache] ← [node memory] ↔ [node memory] → [cache]
- Once everything is in cache, computations are fast

⇒ Trees and graphs for AMR

Challenges in computational sciences

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A history of challenges

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- 7 Physics equations [physics]

Code complexity

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The physicist's view

Implementation and algorithms are technical details.

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The computer scientist's view

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- Compilers can derive equations and do mathematical optimization

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Current approaches

- We tend to do work that should be done by computers
- We bend our physics to make it fit instead of bending languages and compilers
- Compilers can derive equations and do mathematical optimization

What is a programming language?



- S: a set of equations to solve
- T: a number (sequence of 0 and 1) to serve as input of a Turing machine
- f: the morphism computed by the compiler

Code complexity

The physicist's view

Implementation and algorithms are technical details.

The computer scientist's view

The physics is a technical detail.

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- S : a set of equations to solve
- T : a number (sequence of 0 and 1) to serve as input of a Turing machine
- f : the morphism computed by the compiler
- Traditional approach: modifying $S \Rightarrow$ but f can be modified too

A type theory/category theory problem

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Code complexity

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- Parallelism, numerical methods, data structures and physics are all mixed together

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Code complexity

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- Combinatorial explosions of complexity
- Everything but a technical detail
- Boils down to a type theory/category theory problem
- Finding the right abstractions is mostly language independent

Conclusion

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The ideal simulation code

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- Full GR on cosmological scales

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- Should solve $G_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}$ for a given distribution of mass... and that's it

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- Code complexity will come after

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Final remarks

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- Doing Full GR cosmological simulations is aiming for less

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- ... and less is more: more genericity, more correctness, more explainability
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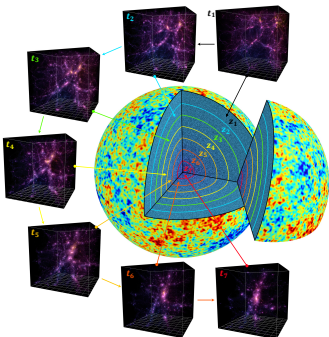
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“Simplicity is the final achievement. After one has played a vast quantity of notes and more notes, it is simplicity that emerges as the crowning reward of art.”

Fryderyk Chopin

Thank you for your attention

Any question?



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