Title: Numerical loop quantum cosmology

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Abstract: In the last decade various cosmological spacetimes have been quantized using the techniques of loop quantum gravity. To understand singularity resolution and decipher reliable Planck scale physics, development of new numerical methods and usage of high performance computing is critical in loop quantum cosmology. In recent years, these developments have robustly demonstrated resolution of singularities in quantum spacetimes. These methods have provided detailed understanding of the emergence of new physics at Planck scale, and of classicality when spacetime curvature becomes very small.Â Further, they have validated an effective spacetime description of the underlying quantum geometry -- a key ingredient of phenomenological predictions in loop quantum cosmology. These lectures will introduce these numerical methods.

Numerical Loop Quantum Cosmology

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Outline

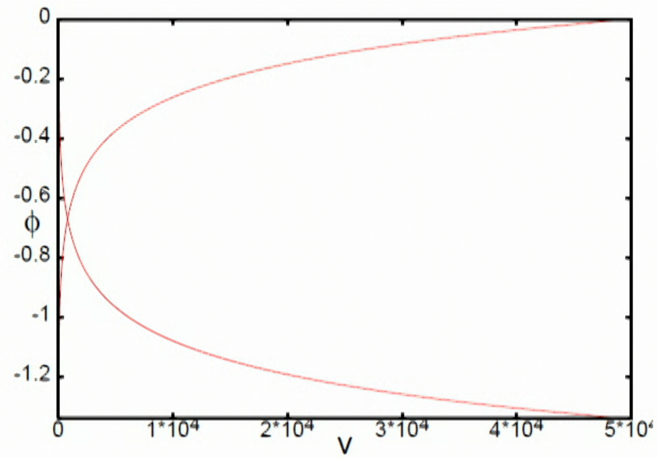
- Introduction to loop quantum cosmology: first results of quantum bounce
- Finite difference methods: gaining insights on different quantizations
- Robustness of quantum bounce and probing deep Planckian geometry
- Summary

A simple example of a big bang

A spatially flat homogeneous and isotropic universe sourced with a massless scalar field ϕ. Matter Hamiltonian: $\mathcal{H}_\phi = P_\phi^2/2v$.

Classically $\rho \propto a^{-6}$. As scale factor $a \to 0$, energy density and curvature become infinite in finite time.

Hamilton's equations give two solutions: an expanding and a contracting universe (both solutions are singular).



Quantum Cosmological Models: WDW approach

- Quantize geometry and matter for a homogeneous universe. Only finite number of degrees of freedom, system can be treated quantum mechanically. Arena to apply the techniques of full theory of quantum gravity in a simplified yet non-trivial setting. (Hope to gain new insights, lessons for full QG).

- Wheeler-DeWitt quantization (based on metric variables) (Misner, Wheeler, DeWitt 1970's):
    - Basic variables: Geometry $\rightarrow v, p_v \propto \dot{v}$, Matter $\rightarrow \phi, p_\phi$.
    - Operators: $\hat{v}\,\Psi(v,\phi) = v\,\Psi(v,\phi)$, $\hat{p}_v\,\Psi(v,\phi) = -i\hbar\frac{\partial}{\partial v}\Psi(v,\phi)$
    - Hamiltonian constraint $\rightarrow (\hat{v}\,\hat{p}_v)^2\,\Psi(v,\phi) = \hat{\mathcal{H}}_\phi\,\Psi(v,\phi)$
    - For a massless scalar in spatially flat isotropic model:

$$12\pi G v \frac{\partial}{\partial v} v \frac{\partial \Psi}{\partial v} = \frac{\partial^2}{\partial \phi^2}\,\Psi(v,\phi)$$

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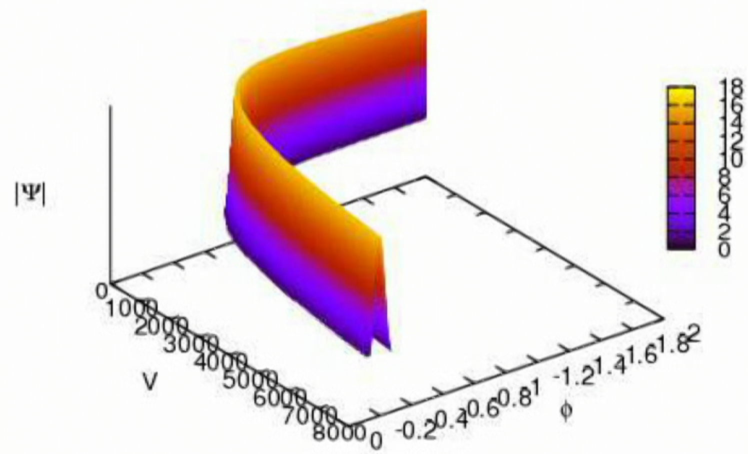
Strategy to extract physics:

- Physical Hilbert space: self-adjoint Hamiltonian constraint, inner product, physical states, observables.
- Construct initial states (such as Gaussian states) in the GR epoch, and evolve them numerically.
- Compute expectation values of observables (and their fluctuations). Compare with the classical trajectory.



WDW states follow the classical trajectory all the way to the big bang. Singularity not resolved.

Loop quantum cosmology

A non-perturbative quantization of homogeneous spacetimes using techniques of loop quantum gravity (Bojowald, Ashtekar, Lewandowski (2001-03)).

LQG based on connection and triad variables which are symmetry reduced before quantization. Captures key elements of the underlying discrete quantum geometry when gravitational part of Hamiltonian constraint expressed in terms of holonomies of the symmetry reduced connection and triads.

$$C_{\rm grav} = -\int_{\mathcal{V}} d^3x\, N\, \varepsilon_{ijk}\, F^i_{ab}\, (E^{aj} E^{bk} / \sqrt{|\det E|})$$

There are different possible regularizations of the field strength. A consistent quantization must be free of fiducial structures, give GR in infra-red limit and should have a well defined scale at which quantum effects become important. In isotropic LQC there is a unique viable quantization (Corichi, Singh (2007)). Von-Neumann stability analysis of quantum Hamiltonian constraint confirms this result (Cartin, Khanna Nelson, Sakellariadou, PS (06-12))

Loop quantization at the level of physical Hilbert space first established for a spatially flat isotropic model with a massless scalar field (Ashtekar, Pawlowski, PS (2006)). Various generalizations available.

Quantum Hamiltonian constraint: $\partial_\phi^2 \Psi = -\Theta\Psi$

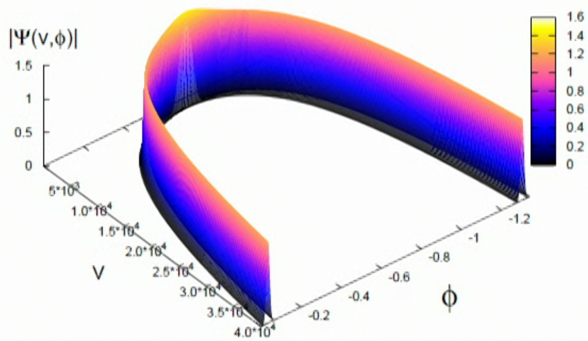
$$\Theta\Psi := -B(v)^{-1}[C^+(v)\Psi(v+4,\phi) + C^o(v)\Psi(v,\phi) + C^-(v)\Psi(v-4,\phi)]$$

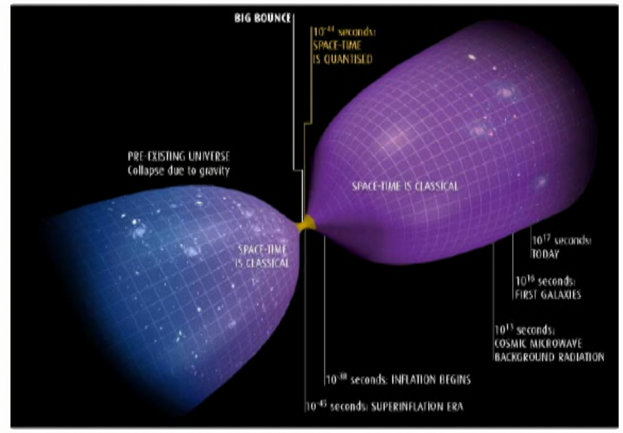
$$\begin{aligned}
C^+(v) &= \frac{3\pi KG}{8}|v+2|\,||v+1|-|v+3||\,, \quad K = \frac{2}{3\sqrt{3\sqrt{3}}} \\
C^-(v) &= C^+(v-4) = \frac{3\pi KG}{8}|v-2|\,||v-3|-|v-1||\,, \\
C^0(v) &= -C^+(v) - C^-(v), \\
B(v) &= \frac{27K}{8}|v|\left||v+1|^{1/3} - |v-1|^{1/3}\right|^3 .
\end{aligned}$$

Discreteness in difference equation a direct manifestation of the non-local nature of the field strength, and the underlying quantum geometry.

At small spacetime curvature (large volume limit), quantum difference equation is approximated by the WDW equation.

Quantum Bounce





Feature Story in New Scientist Dec 2008 by A. Ananthaswamy

For states which are sharply peaked at late times, big bang is replaced by a quantum bounce.

Sharply peaked states bsounce at a maximum of energy density $\rho_{\rm max} = 3/8\pi G\Delta^2 \approx 0.41\rho_{\rm Planck}$

$\Delta \approx 0.29(G\hbar)^{1/2}$ is the minimum area in quantum geometry
Classical singularity recovered when $\Delta \to 0$.

In the last decade, loop quantization of various cosmological spacetimes performed and generalizations studied by various groups. Resolution of singularity found in all the cases.

- Interestingly, for sharply peaked states physics can be captured extremely well by an *effective spacetime* description. Very rich physics explored.
- Impact of bounce studied for signatures in cosmological perturbations in the very early universe (Agullo, Ashtekar, Barrau, Bojowald, de Blas, Grain, Hossain, Maartens, Mena Marugan, Mielczarek, Olmedo, PS, Tsujikawa, ... 2004-15)
- Indications of a potential non-singularity theorem in effective spacetime (Saini, PS 2009-16)

- Techniques applied to black hole spacetimes (Ashtekar, Boehmer, Bojowald, Corichi, Gambini, Modesto, Pullin, Olmedo, PS, Vandersloot 2007-17).
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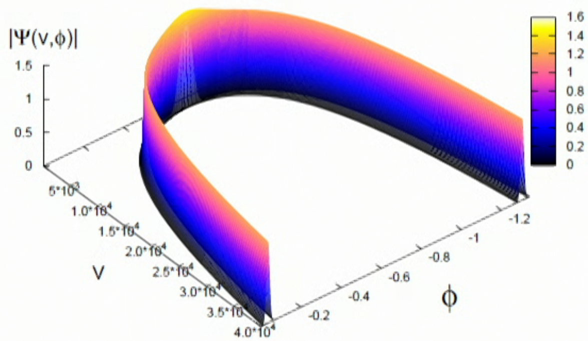

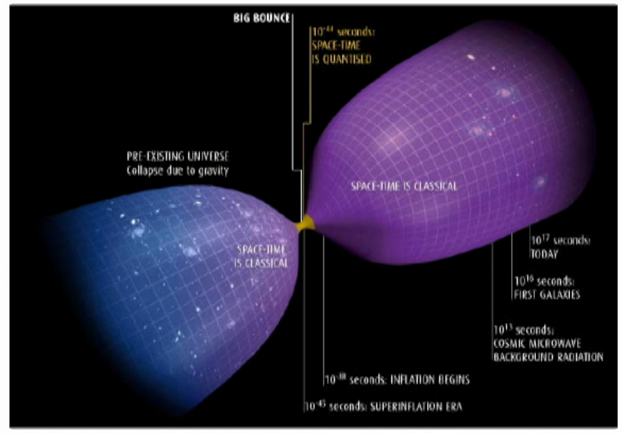

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Many questions remain open

- Is quantum bounce a generic phenomena in the theory?
- Sharply peaked states bounce at volumes greater than $10^3 V_{\text{Planck}}$. For such states effective spacetime description is excellent. But what about quantum states which probe the deep Planck regime? Does effective dynamics still works?
- What is the state of the universe on the other side? How do large quantum fluctuations affect the bounce?
- Do bounces occur in quantum anisotropic models and black hole spacetimes?
- For isotropic model in LQC there is a unique consistent quantization which is physically viable. What about anisotropic models and black hole spacetimes? How do we rule out consistent quantizations?

II. Finite difference methods: Given a discretization, how to determine their viability.

Consider a PDE

$$\frac{\partial v(x,t)}{\partial t} + \frac{\partial f(x,t)}{\partial x} = g(x,t)$$

Depending on complexity of underlying geometry, demand of higher order accuracy and stability, different methods available to obtain a numerical solution.

- Finite difference method
- Finite volume method
- Finite element method: such as continuous and discontinuous Galerkin (DG)

Finite volume and finite element methods are especially well suited for computations in complicated domains on (locally) irregular or unstructured meshes.

The structure of quantum geometry determines which method to use. LQC based on finite difference method, along with applications of DG method in novel algorithms.

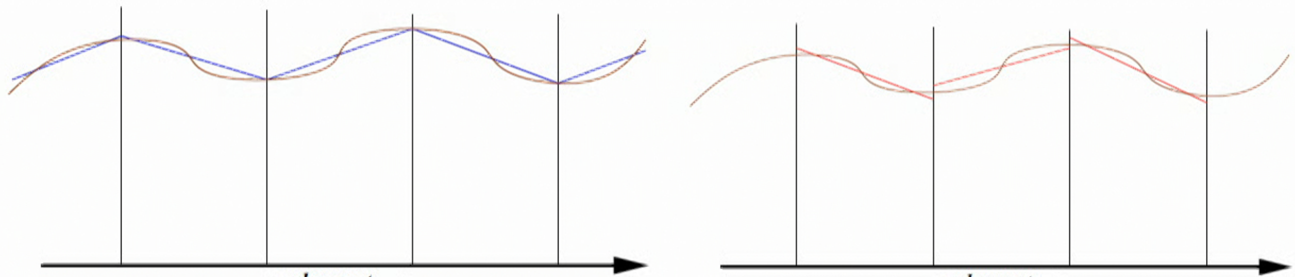
Finite volume and finite element methods

Finite volume: solution approximated in a small volume around a node by a constant $\bar{w}_k(t)$ at the center x_k. PDE is satisfied by the cell average values: $h_k \frac{\mathrm{d}\bar{w}_k}{\mathrm{d}t} + f_{k+1/2} - f_{k-1/2} = h_k \bar{g}_k$.
Divergence term can be evaluated as a surface term. Flux evaluation at the boundary of each finite volume. Powerful method for non-linear conservation laws.

Continuous Galerkin: In each element, local solution is approximated using basis functions $N_i(x_j)$:
$w_h(x) = \sum_{k=1}^{K} w_k N_k(x)$.
PDE can be solved with a continuous Galerkin scheme. Introduce test functions (weak formulation).

$$\int \left(\frac{\partial w_h}{\partial t} + \frac{\partial f_w}{\partial x} - g_w \right) N_i(x) \mathrm{d}x = 0$$

Time implicit scheme. Inversion of a global matrix required.



Continuous Galerkin method *Discontinuous Galerkin method*

In CG method function approximated by a piecewise linear function in each element based on the nodal values.

In DG method on each element we find a piecewise linear discretization. Approximation across the nodes not assumed continuous. Locally continuous discretization, globally discontinuous.

Basis and test functions chosen based on continuous Galerkin, but equation satisfied in sense closer to finite volume.

Resulting matrix local, can be inverted easily. Explicit time scheme. Operators tend to be more sparse than in continuous Galerkin, leading to faster solutions.

Finite differences

Starting from the standard definition

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

we can obtain an approximate numerical derivative making the discreteness of the spatial grid (h) very small.

(i) Forward difference: $\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x+h)-f(x)}{h}$

(ii) Backward difference: $\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x)-f(x-h)}{h}$

(iii) Central difference: $\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x+h)-f(x-h)}{2h}$

Central difference gives more accurate approximation if $h < |f''(x)/f'''(x)|$

Finite difference method

Choose a spatial grid labelled by x_k, with $k = 1..N$. At a grid point x^k , the PDE is approximated using central difference as

$$\frac{\mathrm{d}w(x_k, t)}{\mathrm{d}t} + \frac{f_w(x_{k+1}, t) - f_w(x_{k-1}, t)}{h_k + h_{k-1}} = g(x_k, t)$$

$(h_k = x_{k+1} - x_k)$

w and f_w are numerical approximations to v and f in PDE. These are assumed to be well approximated by local polynomials.

- very simple, highly efficient method
- explicit in time
- extensive theoretical understanding
- unsuitable for complex geometries and discontinuities

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Finite difference method

Consider a hyperbolic PDE

$$\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} = 0$$

To obtain solution, provide initial data $u(0, x)$ at $t = 0$. Determine values of $u(t, x)$ for positive t.

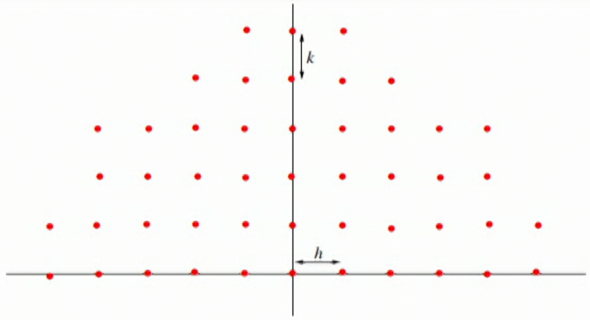
Solution: $u(t, x) = u_o(\xi)$ with $\xi = x - \alpha t$.

Characteristics: lines on which ξ is constant. α is the speed of propagation along the characteristics.

For a system of hyperbolic equations, $\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} + \beta u = g(t, x)$ where u is a vector, characteristic speeds are given by the eigevalues of matrix α (which are real).

Finite difference method

Let us introduce grids in both time and space coordinates, labelled by discreteness h and k respectively. A point (t_n, x_m) is represented as (nk, mh) where n, m are integers.



The hyperbolic PDE can be discretized in various ways utilizing freedom to express derivatives as differences.

Some examples:

Forward time forward space (one step)

$$k^{-1}(w_m^{n+1} - w_m^n) + \alpha h^{-1}(w_{m+1}^n - w_m^n) = 0$$

Leapfrog (multi-step)

$$\frac{1}{2k}(w_m^{n+1} - w_{m-1}^n) + \frac{\alpha}{2h}(w_{m+1}^n - w_{m-1}^n) = 0$$

Consistency and convergence

Using forward time forward space discretization we can write

$$w_m^{n+1} = (1 + \alpha\lambda) w_m^n - \alpha\lambda w_m^{n+1}$$

Here $\lambda = k/h$ is the inverse of the characteristic speed.
The comparison between the solution from finite differencing and the PDE depends on λ and h.

Consistency: a smooth solution of PDE is also a solution of the corresonding finite difference equation.

Convergence: whether solutions of finite difference scheme approximate solutions of the corresonding PDE.

A finite difference scheme may be consistent but not convergent.

Lax-Richtmyer Equivalence Theorem: A consistent finite difference scheme for which initial value problem is well posed is convergent if and only if it is stable.

Stability

Stability of a finite difference scheme leads to restrictions on the way h and k shoud be chosen.

Courant-Friedrichs-Lewy condition: For a hyperbolic equation

$$\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} = 0$$

with an explicit finite difference scheme

$$w_m^{n+1} = a w_{m-1}^n + b v_m^n + c v_{m+1}^n$$

with λ fixed, a necessary condition for stability is $|\alpha\lambda| \leq 1$.

The numerical speed of propagation must be greater than the speed of propagation of PDE $(\lambda^{-1} \geq |\alpha|)$

Courant number: $\nu = \alpha\lambda$. CFL condition implies $|\nu| \leq 1$.