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.

Von Neumann analysis for stability

Using Fourier analysis the finite difference equation:

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

becomes

$$\hat{w}^{n+1} = g(h, \zeta)\hat{w}^n$$

with $g(h, \zeta) = (1 - \alpha\lambda) + \alpha\lambda e^{-i\theta}, \theta = h\zeta$

Advancing the solution by one time step equals multiplying Fourier transform by an amplification factor.

A one step finite difference scheme is stable if and only if $|g(\theta, h, k)| \leq 1 + Ck$ with C as some constant.

If $g(\theta, h, k)$ is independent of h and k, a scheme is stable iff $|g(\theta)| \leq 1$.

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 $|\nu| \leq 1$.

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Example 1: Forward time central space

Finite difference equation:

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

Von-Neumann analysis yields

$$g^n e^{im\theta}\left(g - 1 + \frac{\alpha\lambda}{2}\left(e^{i\theta} - e^{-i\theta}\right)\right) = 0$$

leading to

$$|g|^2 = 1 + \alpha^2\lambda^2\sin^2\theta$$

Hence $|g| > 1$ unless $\theta = 0$ or π.

Forward time central space scheme is unstable. For a fixed α, one can choose λ very small to delay instability. However, instability will apear at a certain time and the solution will blow up.

Example 2: Forward time backward space

Finite difference equation:

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

Von-Neumann analysis yields

$$g^n e^{im\theta}\left(g - 1 + \alpha\lambda(1 - e^{-i\theta})\right) = 0$$

Stability requires $-2\alpha\lambda(1-\alpha\lambda)(1-\cos\theta) \leq 0$

Leads to CFL condition: $|\alpha\lambda| \leq 1.$

If the CFL condition is satisfied the forward time backward space method is stable.

Stability of LQC difference equation at large volume

The quantum Hamiltonian constraint for massless scalar in spatially flat isotropic FRW spacetime can be rewritten as (Ashtekar, Pawlowski, PS (06); Ashtekar, Corichi, PS (08)) (Improved dynamics approach)

$$\partial_\phi^2 \Psi(\nu,\phi) = C_+(\nu)\Psi(\nu+4\lambda,\phi) + C_0(\nu)\Psi(\nu,\phi) + C_-(\nu)\Psi(\nu-4\lambda)$$

where

$$C_+(\nu) = \frac{3\pi G}{4\lambda^2}\,\nu(\nu+2\lambda),\;\; C_-(\nu) = \frac{3\pi G}{4\lambda^2}\,\nu(\nu-2\lambda),\;\; C_0(\nu) = -\frac{3\pi G}{\lambda^2}\,\nu$$

Von-Neumann analysis leads to

$$C_+(\nu)g^2 + (C_0(\nu) - \omega^2)g + C_-(\nu) = 0$$

Amplitude of both roots turn out to be unity.

The quantum Hamiltonian difference equation for improved dynamics is stable at large volumes. (Cartin, Khanna (06))

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Massless scalar + positive Λ in spatially flat isotropic FRW

(Ashtekar, Pawlowski, PS (06), Kaminski, Pawlowski; Pawlowski, Ashtekar (10))

$$\partial_\phi^2 \Psi(\nu, \phi) = C_+(\nu)\Psi(\nu+4\lambda, \phi) + (C_0(\nu) + \pi\gamma^2 G\Lambda\nu^2)\Psi(\nu, \phi) + C_-(\nu)\Psi(\nu-4\lambda)$$

In large volume limit, von-Neumann analysis results in

$$g = \left(1 - 2\frac{\Lambda}{\Lambda_{\rm crit}}\right) \pm \left(\left(1 - 2\frac{\Lambda}{\Lambda_{\rm crit}}\right)^2 - 1\right)^{1/2}$$

where $\Lambda_{\rm crit} := 3/(\gamma^2\Delta)$.

For $0 < \Lambda \leq \Lambda_{\rm crit}$, both roots have magnitude unity.

For $\Lambda > \Lambda_{\rm crit}$, one of the roots has magnitude greater than unity.

von Neumann analysis implies that for $\Lambda > \Lambda_{\rm crit}$, difference equation is not stable at large volumes. (Tanaka et al (11))

Consistent with an independent analysis of the physical Hilbert space (Kaminski, Pawlowski (10))

Stability of earlier LQC quantizations

Massless scalar in spatially flat isotropic FRW (Ashtekar, Bojowald, Lewandowski (03); Ashtekar, Pawlowski, Singh (06))

$$B(p)\partial_\phi^2\,\Psi(\mu,\phi) \;=\; (f_+(\mu)\,\Psi(\mu+4\mu_o,\phi) \;+\; f_0(\mu)\,\Psi(\mu,\phi) \;+\; f_-(\mu)\,\Psi(\mu-4\mu_o$$

where

$$f_+(\mu) \;=\; \frac{1}{2}\sqrt{\frac{8\pi}{6}}\frac{1}{8\pi(\gamma\mu_o)^{3/2}l_{\rm Pl}}\;\left||\mu+3\mu_o|^{3/2}-|\mu+\mu_o|^{3/2}\right|$$

$$f_-(\mu)=f_+(\mu-4\mu_o)\;\;\text{and}\;\;f_0(\mu)=-f_+(\mu)-f_-(\mu)$$

and $B(p)=\left(\frac{6}{8\pi\gamma l_{\rm Pl}^2}\right)^{3/2}\left(\frac{2}{3\mu_o}\right)^6\left(|\mu+\mu_o|^{3/4}-|\mu-\mu_o|^{3/4}\right)^6$

Von-Neumann analysis yields

$$f_+(\mu)g^2+(f_0(\mu)-8\pi GB(p)\hbar^2\omega^2)g+f_-(\mu)=0$$

Both roots have magnitude equal to unity. The difference equation is stable at large volumes. (Nothing seems to be wrong with old loop quantization! Not really.)

Massless scalar + positive Λ in isotropic spatially flat FRW

$$B(p)\,\partial_\phi^2\,\Psi(\mu,\phi) \;=\; f_+(\mu)\,\Psi(\mu+4\mu_o,\phi)\;+$$
$$\left(f_0(\mu)+2\left(\tfrac{8\pi\gamma l_{\rm Pl}^2}{6}\right)^{3/2}\Lambda\mu^{3/2}\right)\,\Psi(\mu,\phi)\;+\;f_-(\mu)\,\Psi(\mu-4\mu_o)$$

von-Neumann stability yields

$$f_+(\mu)g^2+\left(f_0-8\pi G B(p)\,\hbar^2\omega^2+2\left(\frac{8\pi\gamma l_{\rm Pl}^2}{6}\right)^{3/2}\Lambda\mu^{3/2}\right)g+f_-(\mu)=0$$

In the large volume limit we get

$$g_1=0,\quad g_2=-\frac{16\pi}{9}\Lambda\,l_{\rm Pl}^2(\gamma\mu_o)^3\,\mu$$

Since γ and μ_o are fixed by LQG, for any given value of Λ, there exists a sufficiently large value μ, such that $|g_2|>1$. The quantum difference equation is unstable. Not a viable quantization.

III. Robustness of bounce

Numerical challenges

The quantum difference equation is extremely well approximated by the second order Wheeler-DeWitt differential equation at small spacetime curvatures (large volumes).

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

Characteristic speeds: $\lambda^{\pm} = \pm\sqrt{12\pi G}v$

The stability of evolution constraints the maximum time step $\Delta\phi$:

$$\Delta\phi \leq \frac{\Delta v}{|\lambda^{\pm}|} \propto \frac{1}{v}$$

Volume discreteness is fixed. The maximal possible time step is inversely proportional to the maximal volume on the grid.

States which are highly quantum, and which probe deep Planckian geometry require a very large grid in volume. The computational cost of such numerical simulations is extremely high.

Numerical challenges for isotropic and anisotropic models

- Isotropic models:
  - For sharply peaked initial states simulations: $v_{\rm outer} \sim 10^5$, computational time $\sim$ 15 minutes on single core.
  - For widely spread states and those which can probe deep Planck regime, $v_{\rm outer} \sim 10^{12}$ (and higher). This requires 10^7 more spatial grid points. Since quantum grid is fixed, stability requirements lead to 10^7 finer time steps. Such a simulation would take 10^{10} years!

- Anisotropic models:
  - Non-hyperbolicity encountered for Bianchi-I vacuum model when casted in relational observables. However, one can evaluate the entire physical wavefuntion by integration

$$\chi(b_1, v_2, v_3) = \int d\omega_2 d\omega_3 \tilde{\chi}(\omega_2, \omega_3) e_{\omega_1}(b_1) e_{\omega_2}(v_2) e_{\omega_3}(v_3)$$

  - For a state sharply peaked at $\omega_2 = \omega_3 = 10^3$, a typical simulations require 10^{14} floating point operations.
  - For wider states, and states probing deep quantum geometry, typical simulations require 10^{19} flop. Memory needed $\sim$ 5 Tb.

Chimera scheme

(Diener, Gupt, PS (2014))

- Exploits the agreement between LQC and WDW theory at large volumes.
- Use two grids: An inner grid where the LQC difference equation is solved, and a carefully chosen outer grid at large volumes where the WDW theory is an excellent approximation.
- WDW equation is a partial differential equation, and we can choose a different discretization in the outer grid using FD or DG methods.
- Choose a new coordinate: $x = \ln v$

$$\frac{\partial^2 \Psi}{\partial \phi^2} = 12\pi G v \left(\frac{\partial}{\partial v} \left(v \frac{\partial \Psi}{\partial v} \right) \right) = 12\pi G \frac{\partial^2 \Psi}{\partial x^2}.$$

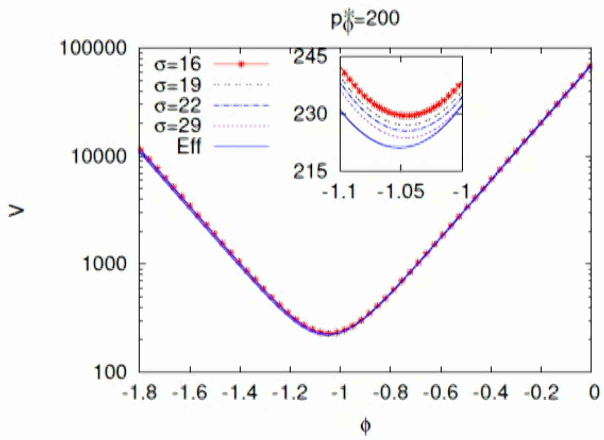
- Characteristic speeds are constants: $\lambda^{\pm} = \pm\sqrt{12\pi G}$.

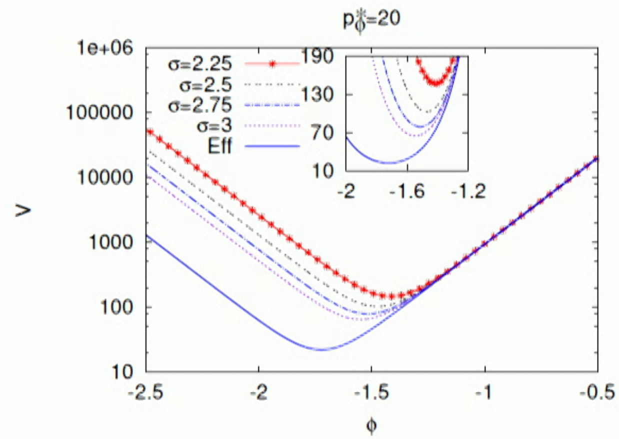
With the Chimera scheme with $v_{\rm int} = 12,500$ and $v_{\rm outer} = 2 \times 10^{12}$ the evolution takes only 5 minutes on a single core.

Results: Testing the validity of effective description

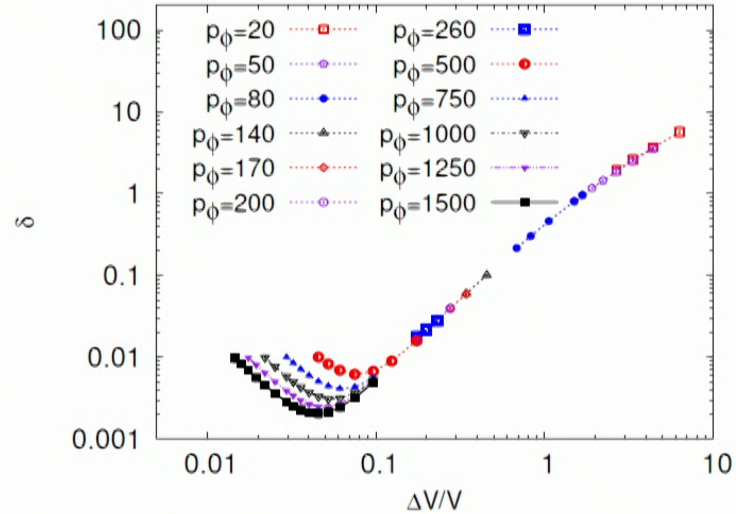
At a coarse level, effective theory captures underlying quantum evolution quite well, especially for sharply peaked states.

However, effective theory becomes less reliable for states which bounce deeper in Planck regime (even if $v \gg 1$), and for states which have wide spreads **(Diener, Gupt, PS (2014))**





Departures of effective description from the quantum evolution found to depend in a subtle and non-monotonic way on the values of field momentum and fluctuations.



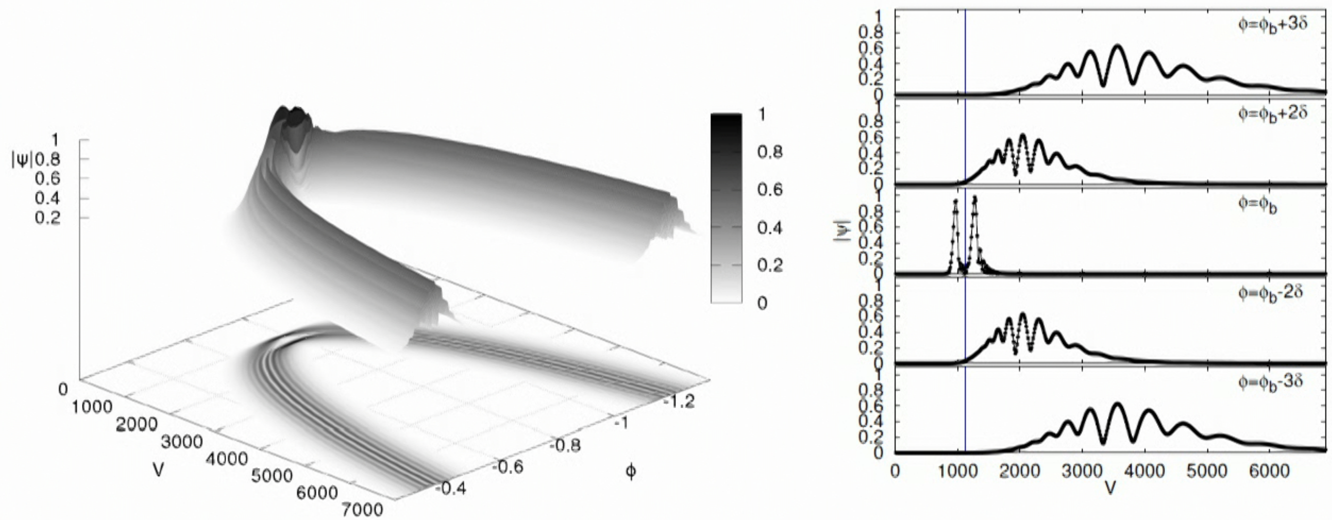
As an example, contrary to heuristic expectations, it is not always true that for smaller relative fluctuations effective theory captures quantum evolution better.

Nature of the departures also found to be quite sensitive to the construction of initial states. Extra care needed in reaching generalized conclusions in the effective descriptions.

Quantum bounce for highly quantum states

Bounce not restricted to any special states. Even occurs for states which are highly non-Gaussian or squeezed.

(Diener, Gupt, Megevand, PS (2014))



Tight constraints on the growth of the fluctuations across the bounce. State in the asymptotic future turns out to be very similar to the one in the asymptotic past. Results are in agreement with earlier analytical estimates (Corichi, Kaminski, Montoya, Pawlowski, PS (2008-11))

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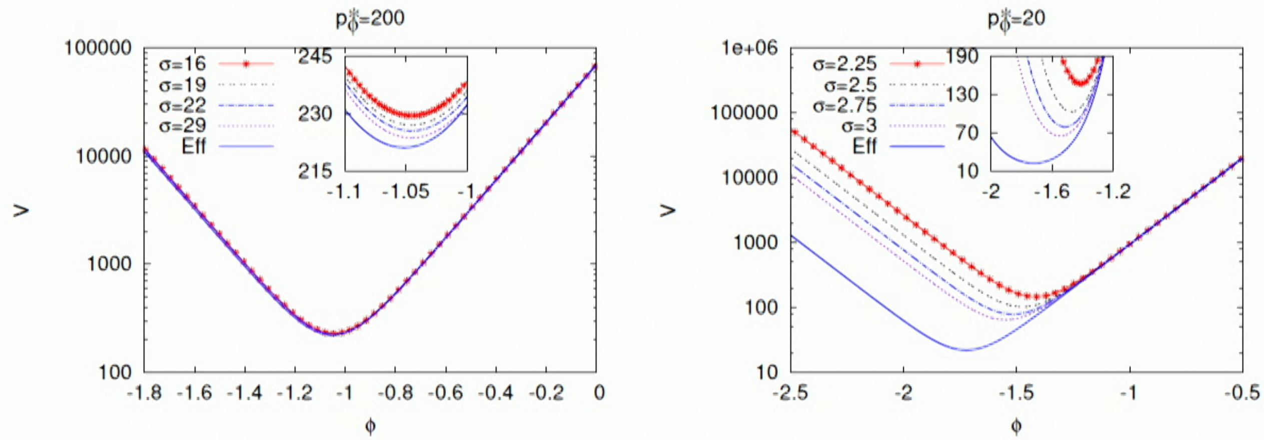
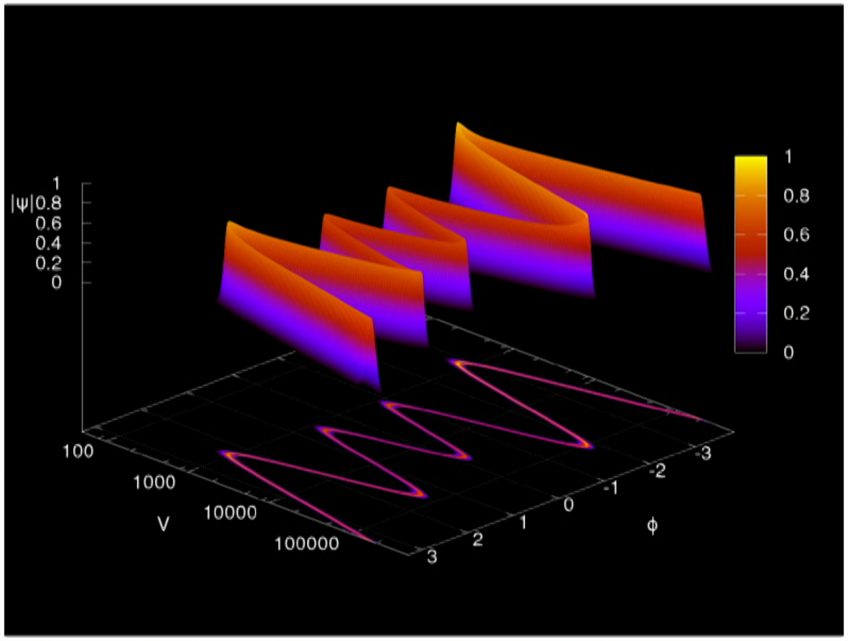


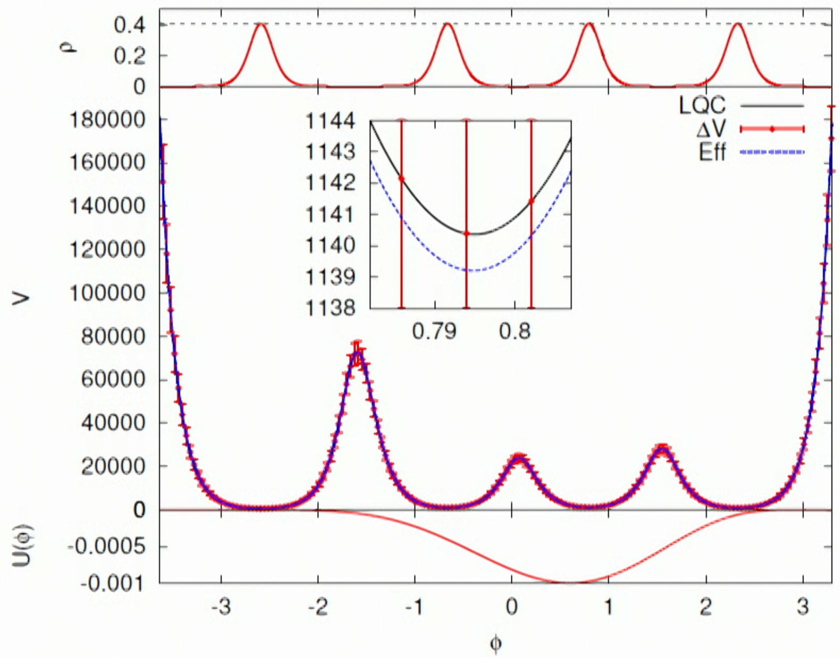
Cyclic model inspired potential

Potential: $U = U_o e^{-\phi^2}$ (Diener, Gupt, Megevand, PS (appearing soon))



Quantum bounce occurs even in the presence of a steep potential. Qualitative features of the bounce unaffected by the potential for various choices of parameters and initial conditions.

Effective description in very good agreement in the presence of potential for sharply peaked states.



Evolution can be asymmetric across the multiple bounces. State remains sharply peaked through out the evolution.

Non-singular evolution also achieved in inflationary potentials

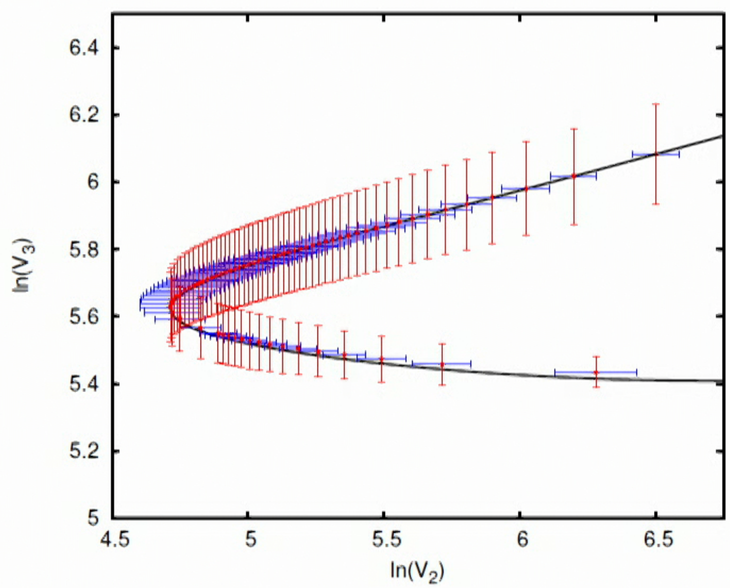
(Ashtekar, Pawlowski, PS (in progress))

Anisotropic quantum bounce

Rigorous quantization of Bianchi-I vacuum model available. Singularity resolution found (Martin-Benito, Mena Marugan, Pawlowski (2008)).

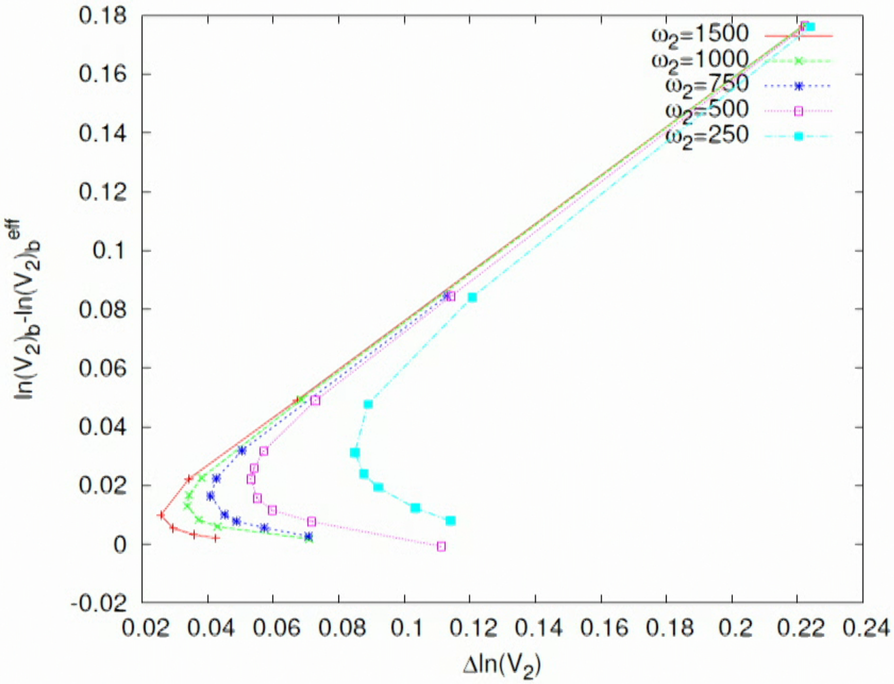
Cactus implementation of the Bianchi-I vacuum spacetime performed. Using HPC we can now rigorously understand the physics of quantum bounce in Bianchi-I vacuum

(Diener, Joe, Megevand, PS (2017))



Effective description turns out to be a good approximation for sharply peaked states in the Bianchi-I model.

As in the isotropic model, the agreement between the quantum evolution and the effective theory depends non-monotonically on the relative fluctuations.



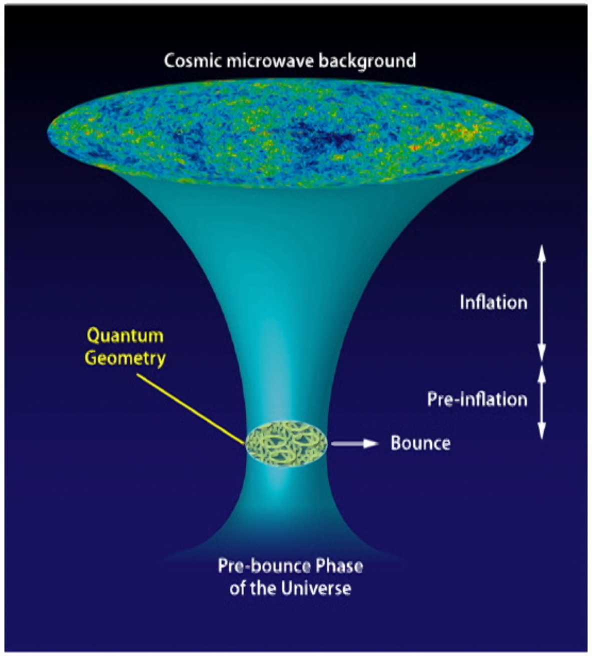
Summary

- Quantum geometry provides a glimpse on the way big bang singularity may be resolved. No need of exotic matter/fine tuning.
- With new numerical algorithms and using HPC, we are now able to explore extreme regimes of the quantum spacetime.
- Numerical simulations prove to be an invaluable tool to extract detailed physics of the quantum spacetime.
- Quantum bounce turns out to be a generic feature in all the simulations performed so far, including for highly quantum states, in presence of potentials and anisotropies.
- Using numerical simulations, valuable insights gained on the validity of effective descriptions and when can the resulting physics be considered reliable.

Future Directions

For some cosmological models, physics of quantum geometry established with caveats (discovered computationally).

But for more general models, such as in presence of inflation, anisotropies and inhomogeneities, most of the physics unexplored. Many analytical and conceptual issues need to be overcome while numerical hurdles are crossed.



P. Singh, Physics 5, 142 (2012)

In the next decade, computational methods in quantum gravity must for extracting robust predictions about the reliable signatures of quantum geometry, such as in CMB.