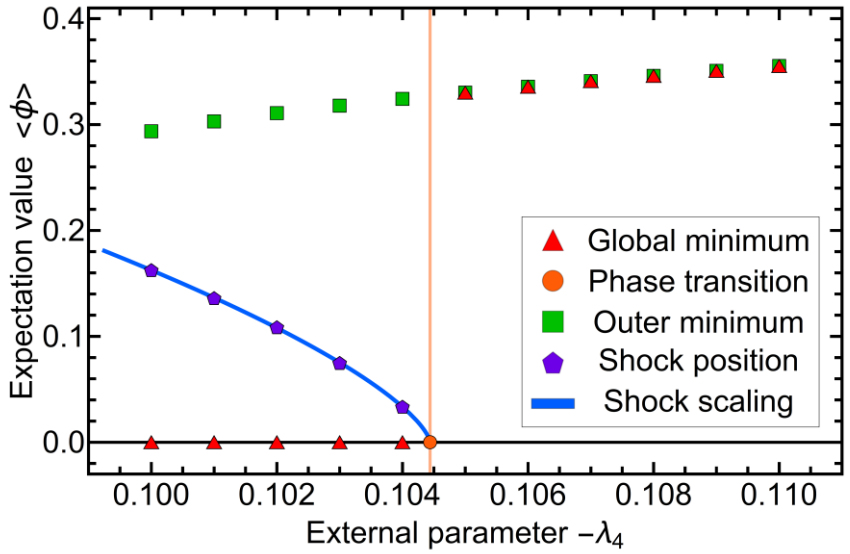
Resolving phase transitions with Discontinuous Galerkin methods

Functional Methods in Strongly Correlated Systems



Nicolas Wink

Work in collaboration with:

Eduardo Grossi

Jan M. Pawlowski

Grossi, NW, arxiv:1903.09503

Grossi, Pawlowski NW, in prep.

Partial differential equations

Partial differential equations of interest:

For simplicity: $u(t,x)$
scalar with one spatial dimension

$$\partial_t u \; + \; \partial_x f^{(c)}(u,t,x) \; + \; \partial_x f^{(D)}(u,\partial_x u,t,x) \; = \; s(u,t,x)$$

Conservation term (Goldstone modes) — Diffusion term (Radial mode) — Source term (Fermions)

A lot of physical systems are described (partially) by this class of equations:

- Maxwell equations
- General relativity + Magneto Hydro
- Navier–Stokes equations
- Functional renormalization Group equations

Discontinuous Galerkin methods are designed precisely designed for this set of equations

Conservation laws

Consider only the scalar conservation law

$$\partial_t u + \partial_x f(u) = 0$$

Given numerical approximations

$$u_h(t, x_k) \quad \text{and} \quad f_h(u_h(t, x_k))$$

Several options how the residual should vanish

$$\mathcal{R}_h = \partial_t u_h + \partial_x f_h = 0$$

On each node of the mesh:

$$\Rightarrow \mathcal{R}_h(t, x_k) = 0$$

- Finite difference methods
- Finite volume methods
- ….

Residual orthogonal to all test functions in some space:

$$\Rightarrow \int_\Omega \mathcal{R}_h(t, x)\phi_h(x) = 0$$

- Finite element methods
- Spectral methods
- …

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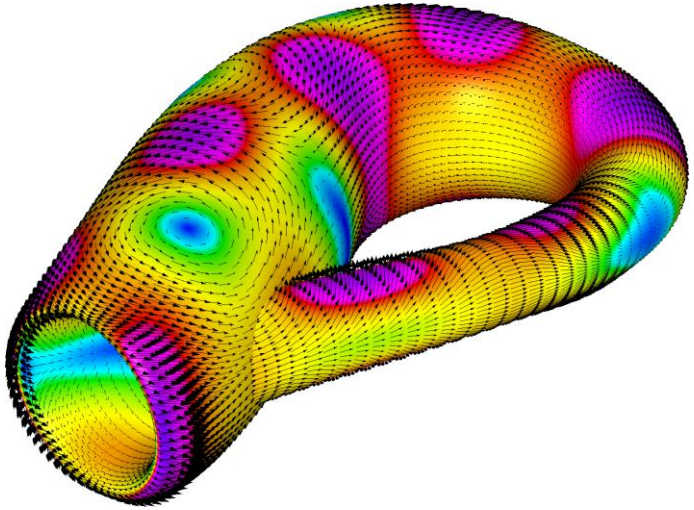

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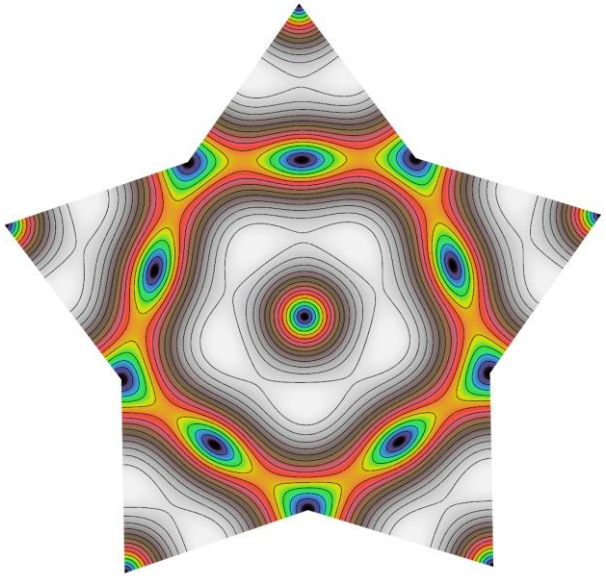
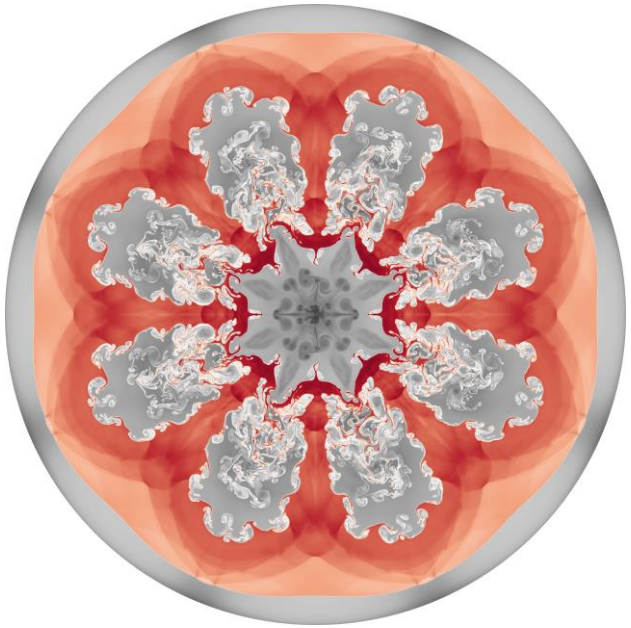


Discontinuous Galerkin methods



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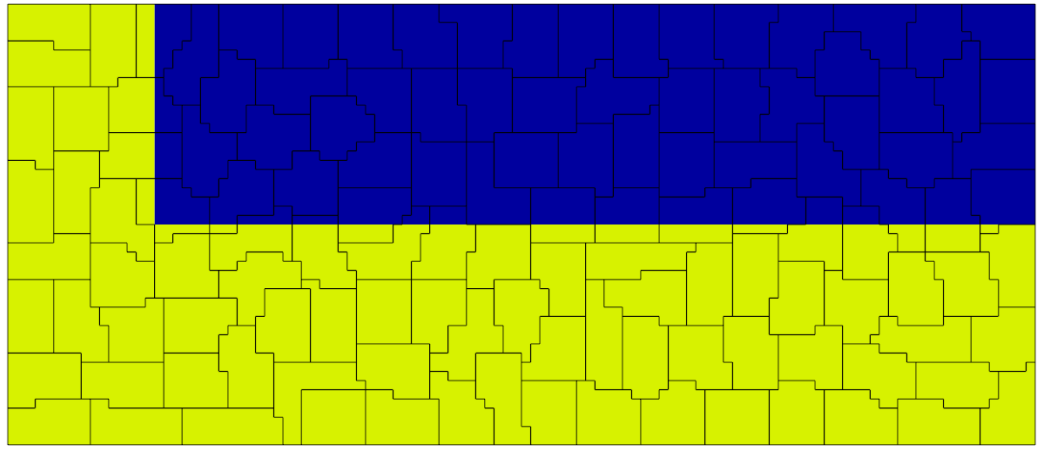

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The basic idea

The method combines two basic ideas:

$$\mathcal{R}_h(t, x_k) = 0$$

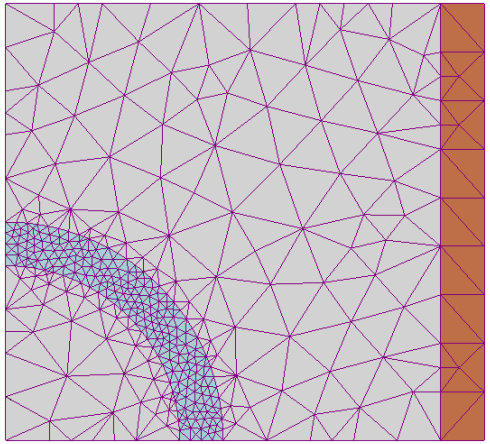
$$\int_\Omega \mathcal{R}_h(t, x)\phi_h(x) = 0$$

Finite volume methods

- Residue vanishes for cell averages
- Local & geometric flexible
- Inherently discontinuous
- Higher order accuracy problematic

Finite element methods

- Residue vanishes in a weak sense
- High order accuracy & geometric flexible
- Usually continuous
- Method is “global” (one giant matrix)



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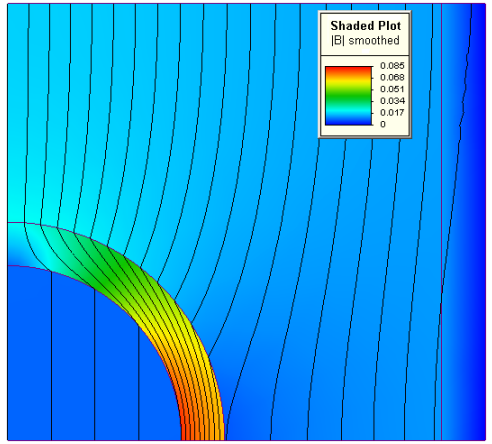
Take the best from both

➡ Discontinuous Galerkin methods

Slightly more technical: An extension of finite element methods that reduces to finite volume schemes at lowest order



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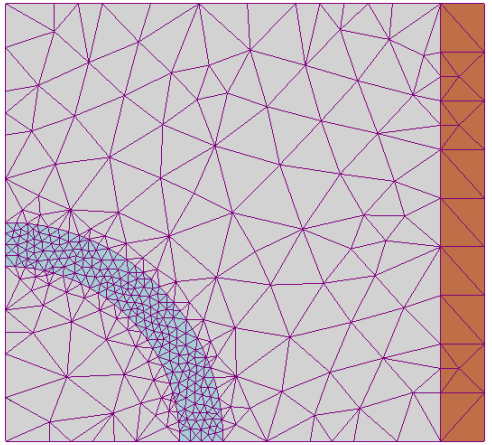
Local approximation

Approximate solution over computational domain

$$\Omega \simeq \Omega_h = \bigcup_{k=1}^{K} D^k$$



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$$u(t,x) \simeq u_h(t,x) = \bigoplus_{k=1}^{K} u_h^k(t,x)$$

Expand the solution in each element in a local polynomial basis of degree N

$$u_h^k(t,x) = \overbrace{\sum_{n=1}^{N+1} \hat{u}_n^k(t)\psi_n(x)}^{\text{Modal expansion}} = \overbrace{\sum_{i=1}^{N+1} u_h^k(t,x_i^k) l_i^k(x)}^{\text{Nodal expansion}}$$

Modes

(Orthogonal) polynomial basis

Nodes

Associated Lagrange polynomial

Good choice (obviously) important

- Legendre polynomials
  ➡ Spectral convergence
- Gauss-Lobatto points
  ➡ Ensures well conditioning while switching between bases

Hesthaven, Warburton, Nodal Discontinuous Galerkin Methods (2008)

Weak formulation

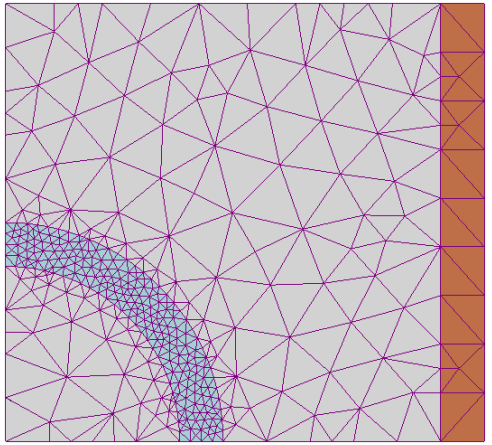
$$\int_{D^k} \left(\partial_t u_h^k + \partial_x f_h^k(u_h^k)\right)\psi_n \, \mathrm{d}x = 0$$

Discontinuous elements:
More degrees of freedom than equations!

Partial integration

$$\int_{D^k} \left(\left(\partial_t u_h^k\right) \psi_n - f_h^k(u_h^k)\partial_x \psi_n \right) \mathrm{d}x = - \int_{\partial D^k} \hat{\mathbf{n}} \cdot f^* \psi_n \, \mathrm{d}x$$

Weak form



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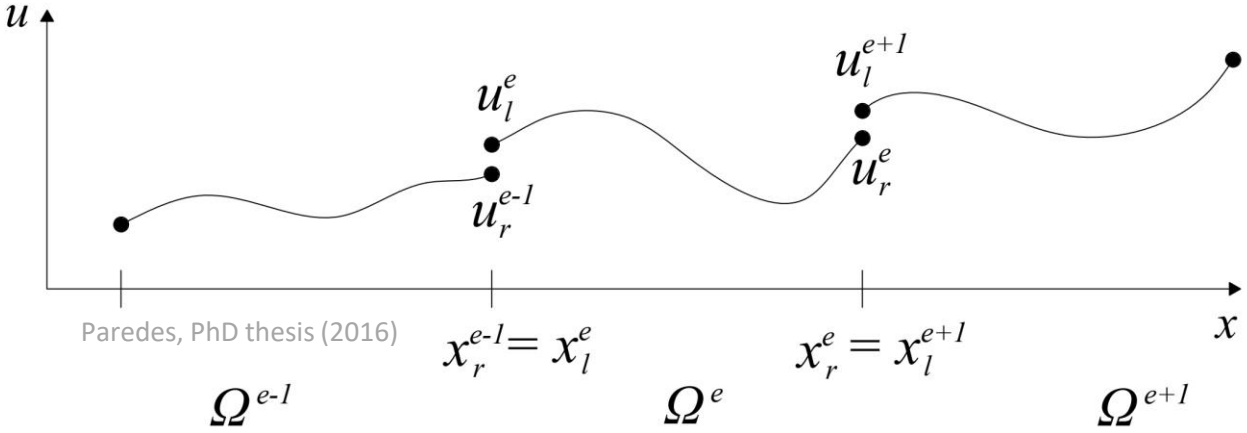
<u>Numerical flux</u>

Connects elements (closes set of equations)



Paredes, PhD thesis (2016)

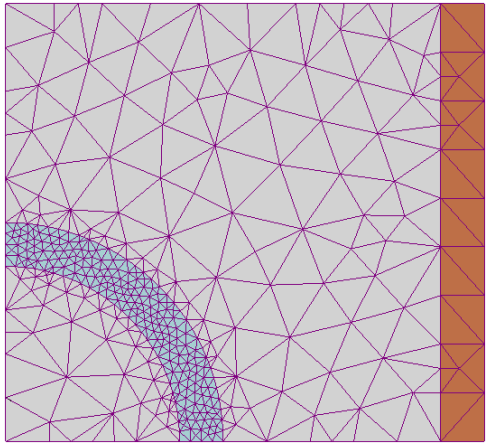
Hesthaven, Warburton, Nodal Discontinuous Galerkin Methods (2008)

Numerical flux

Numerical flux

$$\int_{D^k} \left(\partial_t u_h^k + \partial_x f_h^k(u_h^k)\right)\psi_n \, \mathrm{d}x = \int_{\partial D^k} \hat{\mathbf{n}} \cdot \left(f_h^k(u_h^k) - f^*\right) \psi_n \, \mathrm{d}x$$

Strong form



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- Restricted by rather general conditions (consistency, …)
- Defines how to treat a jump discontinuity between elements
- Acts physically like a tiny dissipation
- A variety of choices available

Constant related to the propagation speed of information

$$C \geq \max_{D^{\{i,i\pm1\}}} |\partial_u f(u)|$$

Lax-Friedrichs flux

$$f^*(u_h^-, u_h^+) = \{\{f_h(u_h)\}\} + \frac{C}{2}[\![u_h]\!]$$

$$\{\{f\}\} = \frac{1}{2}\left(f^- + f^+\right)$$

Average

$$[\![u]\!] = \hat{\mathbf{n}}^- u^- + \hat{\mathbf{n}}^+ u^+$$

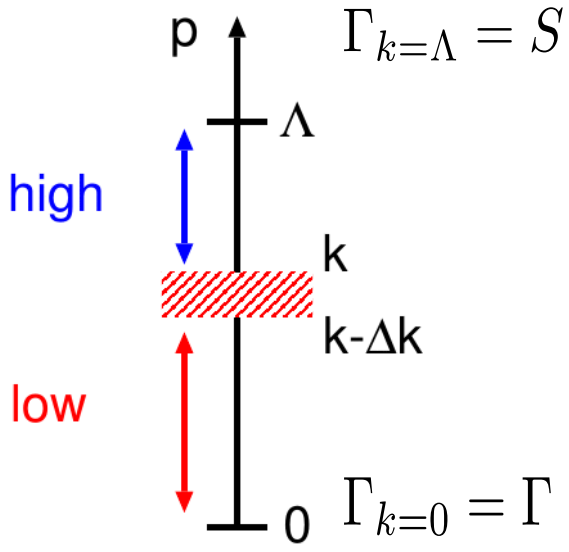
Difference

Usually an efficient, accurate and robust choice

Hesthaven, Warburton, Nodal Discontinuous Galerkin Methods (2008)

Functional Renormalization Group

Functional Renormalization Group



- Non-perturbative first principle method
- Systematically integrate out momentum shells
- Access to physical mechanisms
- No sign problem
  - Chemical potential
  - Real time

Wetterich equation:

$$\partial_t \Gamma_k[\phi] = \frac{1}{2} \mathrm{Tr} \frac{1}{\Gamma_k^{(2)}[\phi] + R_k} \partial_t R_k$$

RG-time:

$$t = -\ln \frac{k}{\Lambda}$$

Momentum scale

Reference scale
(set to 1 here)

Integrating theory from $t = 0$ to $t = \infty$ includes all quantum effects

O(N) - Model

O(N) - Model

Relevant in many physical settings:

- (Pseudo)-scalar sector in QCD
- Higgs potential
- Condensed matter
- …

N-component scalar theory with classical action:

$$S = \int_x \left\{ \frac{1}{2}(\partial_\mu \phi_a)^2 + \lambda_2 \phi_a \phi^a + \lambda_4 (\phi_a \phi^a)^2 + \lambda_6 (\phi_a \phi^a)^3 \right\}$$

Invariant: $\rho = \frac{1}{2}\phi_a \phi^a$

→ Finite field expectation value signals spontaneously broken symmetry

Lowest order approximation in a derivative expansion, LPA:

$$\Gamma_k = \int_x \left\{ \frac{1}{2}(\partial_\mu \phi_a)^2 + V(\rho) \right\}$$

$\xrightarrow[\text{Rescale with (N-1)}]{\text{Flow equation}}$

$$\partial_t V(\rho) = \frac{\Omega_d}{(2\pi)^d} \frac{(\Lambda e^{-t})^{d+2}}{d} \left(\frac{1}{(\Lambda e^{-t})^2 + V'(\rho)} + \frac{1}{N-1} \frac{1}{(\Lambda e^{-t})^2 + V'(\rho) + 2\rho V''(\rho)} \right)$$

Connecting to DG

Flow equation for the effective potential:

$$\partial_t V(\rho) = \frac{\Omega_d}{d(2\pi)^d} \frac{(\Lambda e^{-t})^{d+2}}{(\Lambda e^{-t})^2 + V'(\rho)}$$

Not ideally suited for numerical applications

Introduce new variable for the derivative:

$$u(\rho) = \partial_\rho V(\rho)$$

RHS now defines a flux:

$$f(t,u) = -\frac{\Omega_d}{d(2\pi)^d} \frac{(\Lambda e^{-t})^{d+2}}{(\Lambda e^{-t})^2 + u}$$

$$\partial_t u + \partial_\rho f(t,u) = 0$$

Standard conservative form

Initial & Boundary conditions:

$$u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$$

Allows for access to first & second order phase transitions

- We require a solution on $\rho \in [0, \rho_{\max}]$
- Boundary conditions required for inflow boundary conditions $\hat{\mathbf{n}} \cdot (\partial_u f) < 0$

Boundary condition at large field values required, but naturally suppressed for physical potentials

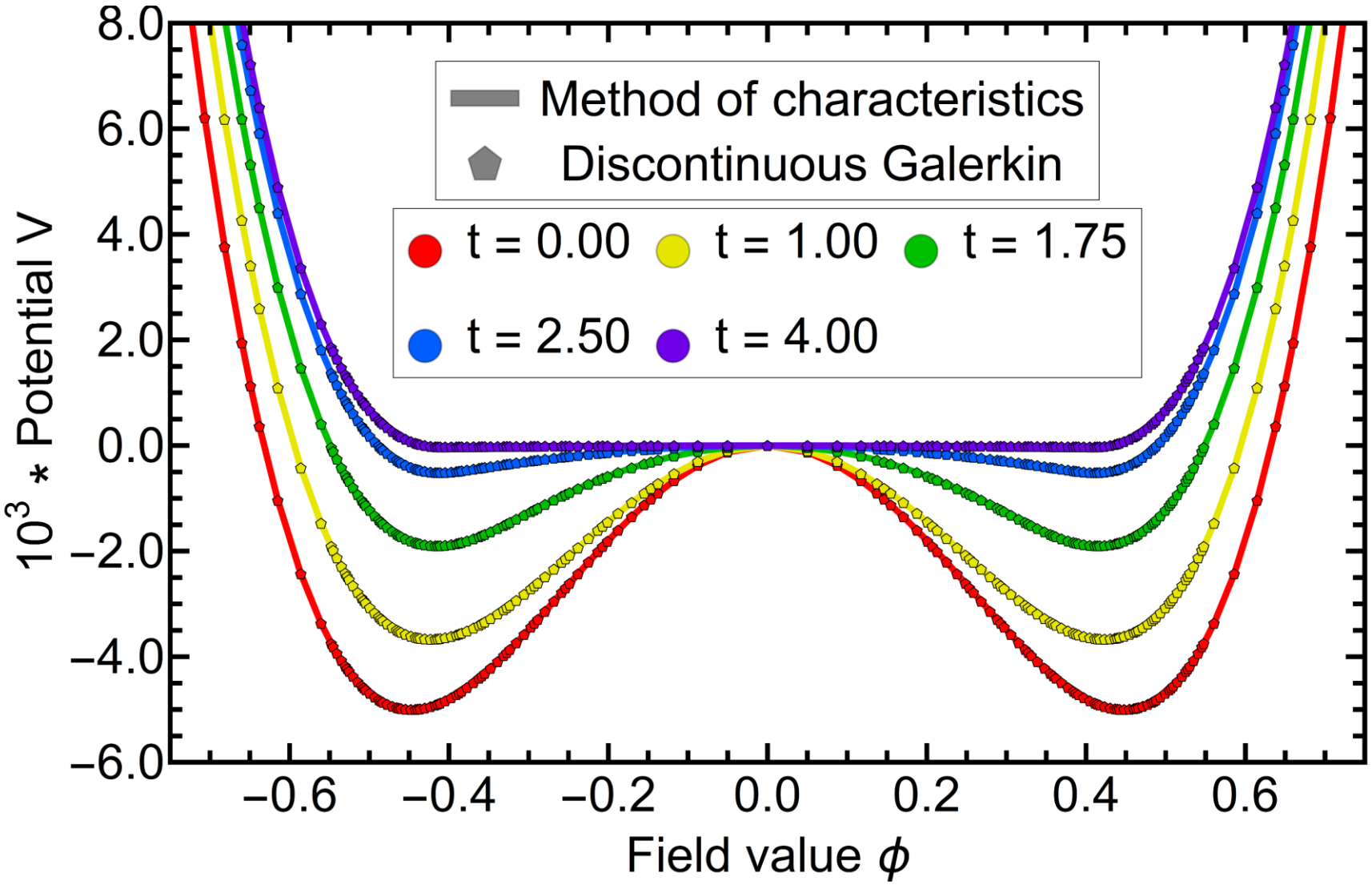
Together with $d = 3$ and $\Lambda = 1$

Grossi, NW, arxiv:1903.09503

Second order phase transition

Potential

Initial condition: $u(t=0) = -\frac{1}{10} + \rho$

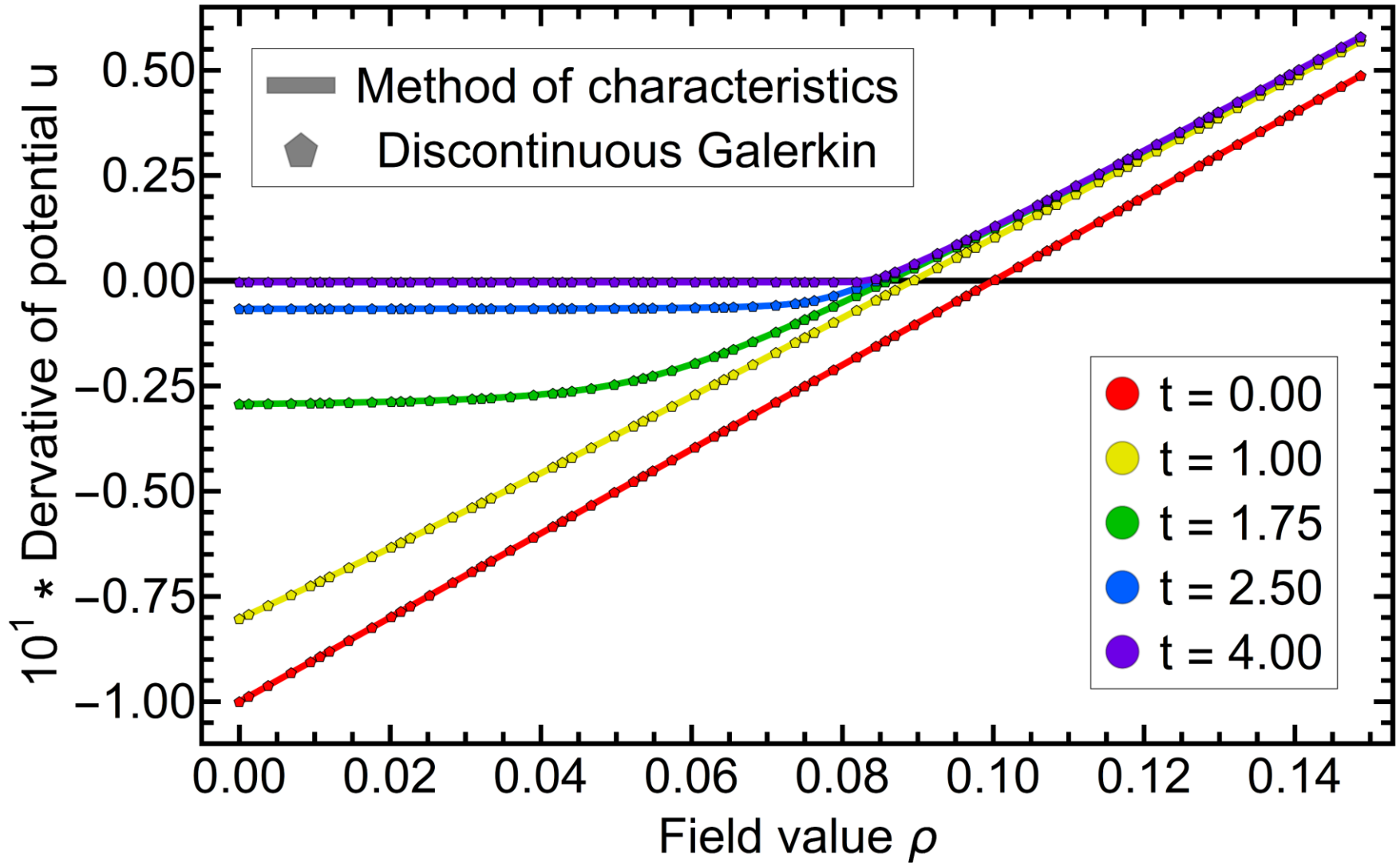


Calculated with N=5, K=30

Grossi, NW, arxiv:1903.09503

Derivative

Initial condition: $u(t=0) = -\frac{1}{10} + \rho$



- Zero crossing signals position of minimum

  ⇓

  Example of symmetry broken phase

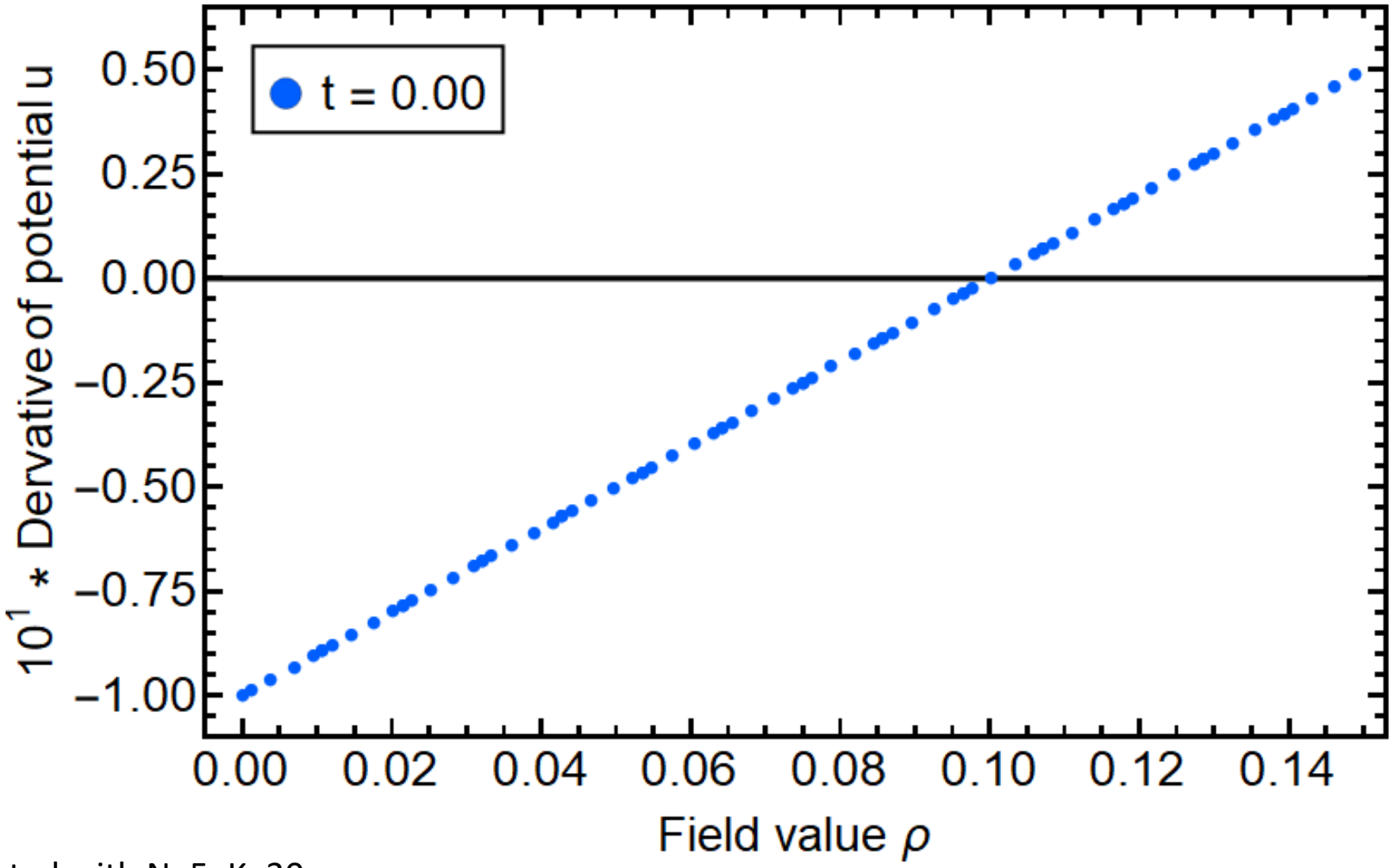
- Convexity restoration nicely visible

Calculated with N=5, K=30

Grossi, NW, arxiv:1903.09503

Derivative

Initial condition: $u(t=0) = -\frac{1}{10} + \rho$



- Zero crossing signals position of minimum

  ⇓

  Example of symmetry broken phase

- Convexity restoration nicely visible

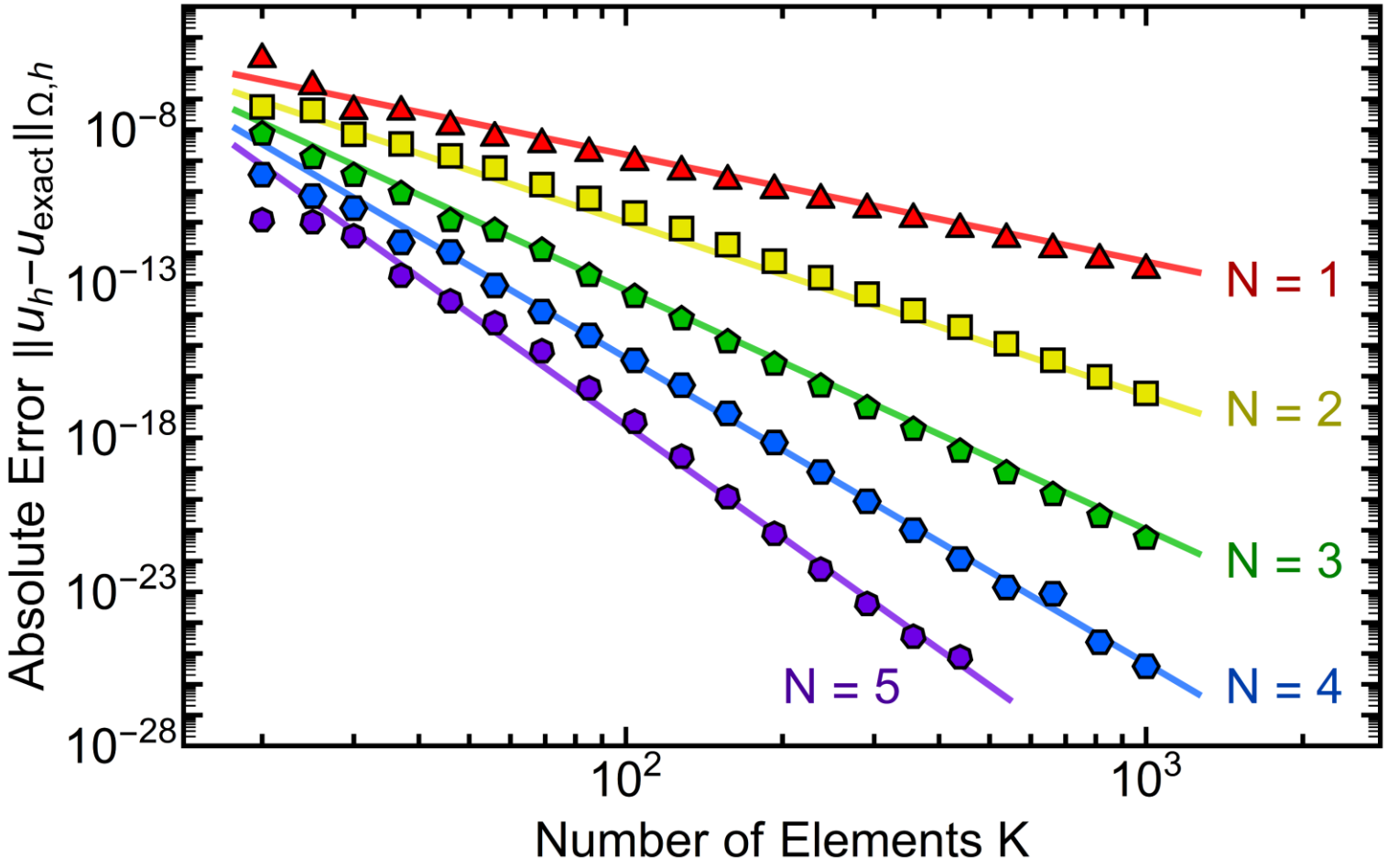
Calculated with N=5, K=30

Grossi, NW, arxiv:1903.09503

Convergence

Initial condition: $u(t=0) = -\frac{1}{10} + \rho$

25 order of magnitude!

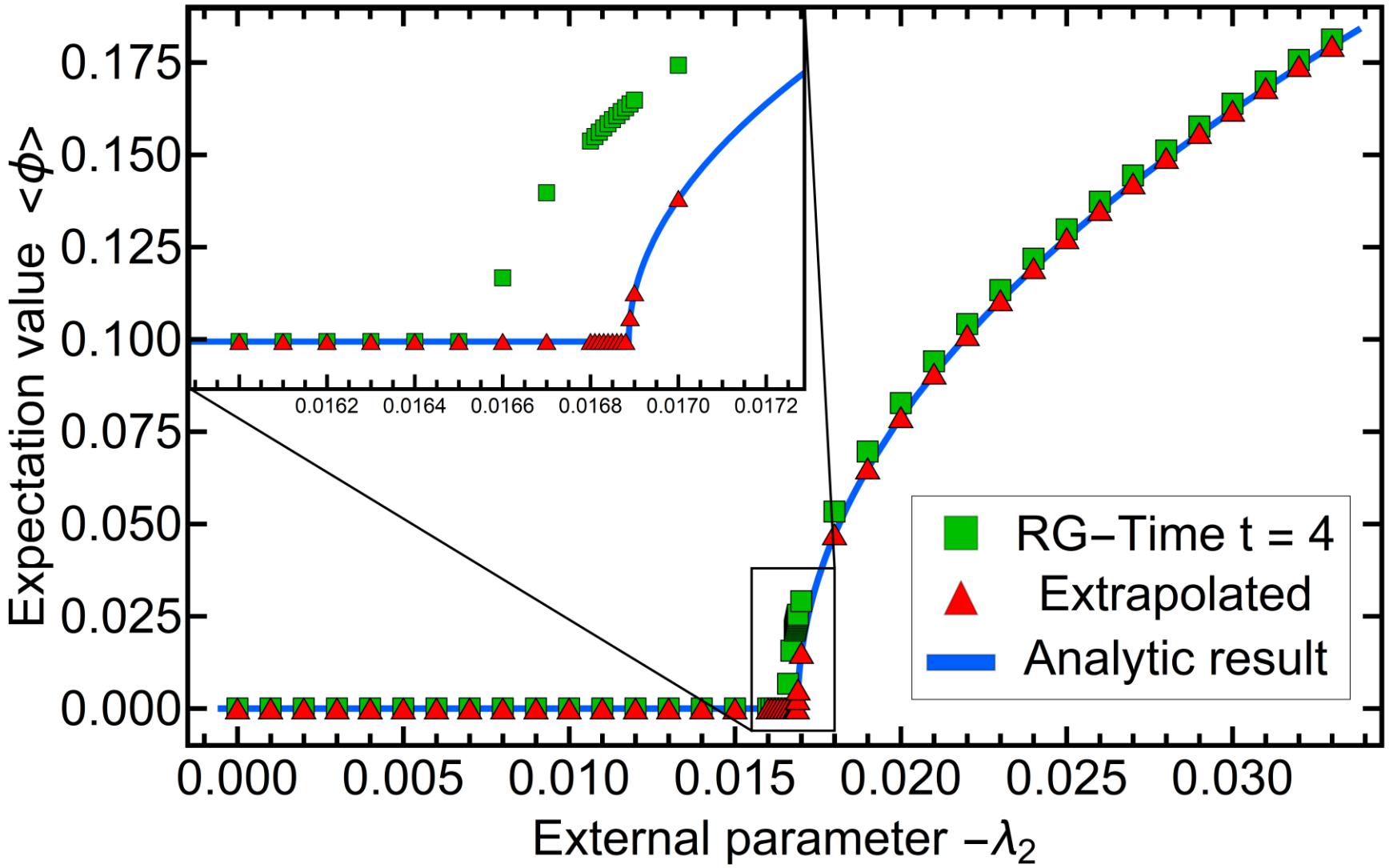


- t=1.75 (already kink like)
- Power law in number of elements
- Spectral convergence in local approximation order
- Lines from a single fit

Grossi, NW, arxiv:1903.09503

Phase transition

Initial conditions: $u(t=0) = \lambda_2 + \rho$



- Second order phase
- Critical exponent agrees with mean field (within error)
- Extrapolation to infinite time easily possible

Calculated with N=5, K=120

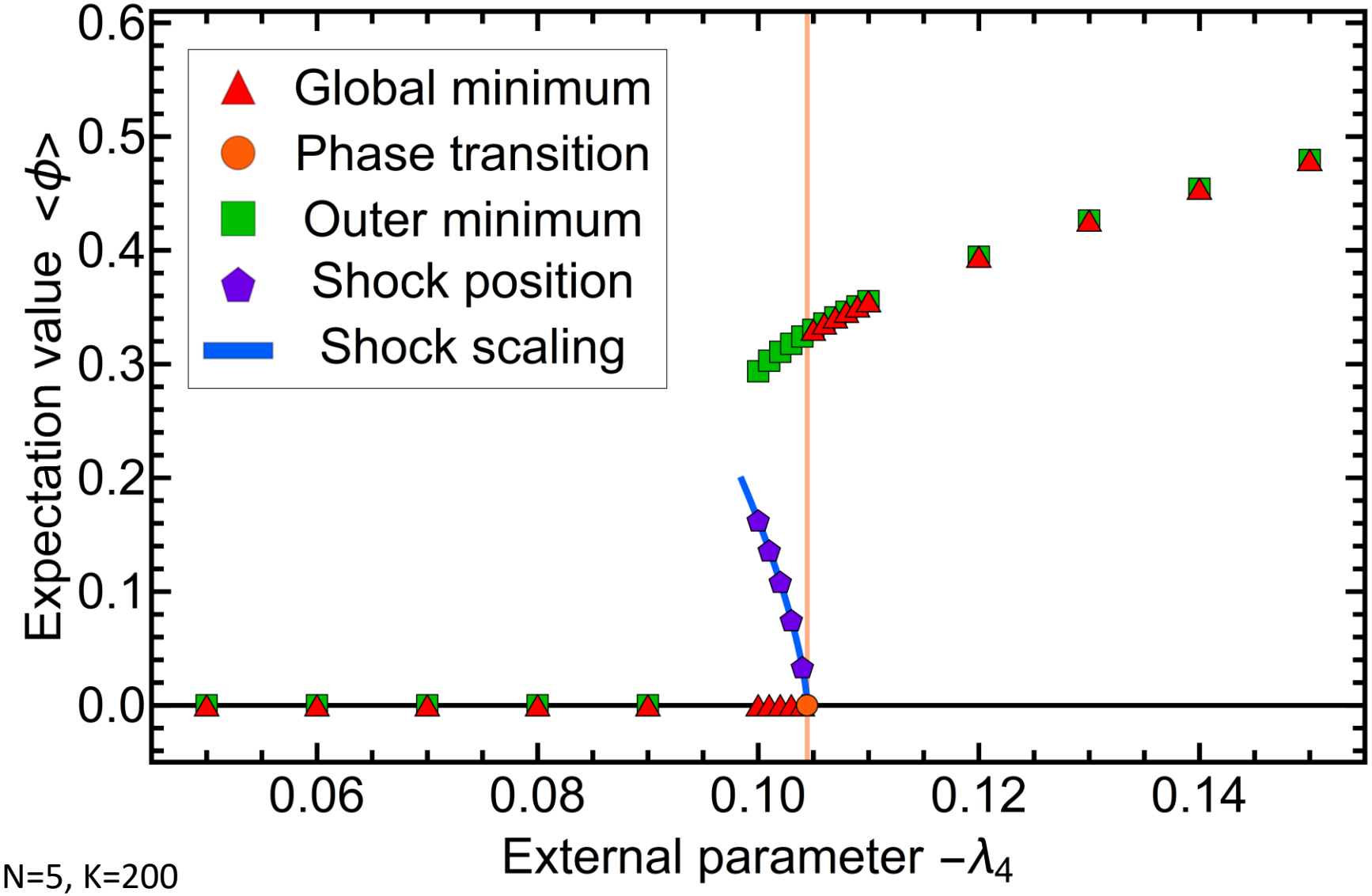
Grossi, NW, arxiv:1903.09503

First order phase transition

1st-order phase transition

Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$

with $\lambda_4 < 0$



Calculated with N=5, K=200

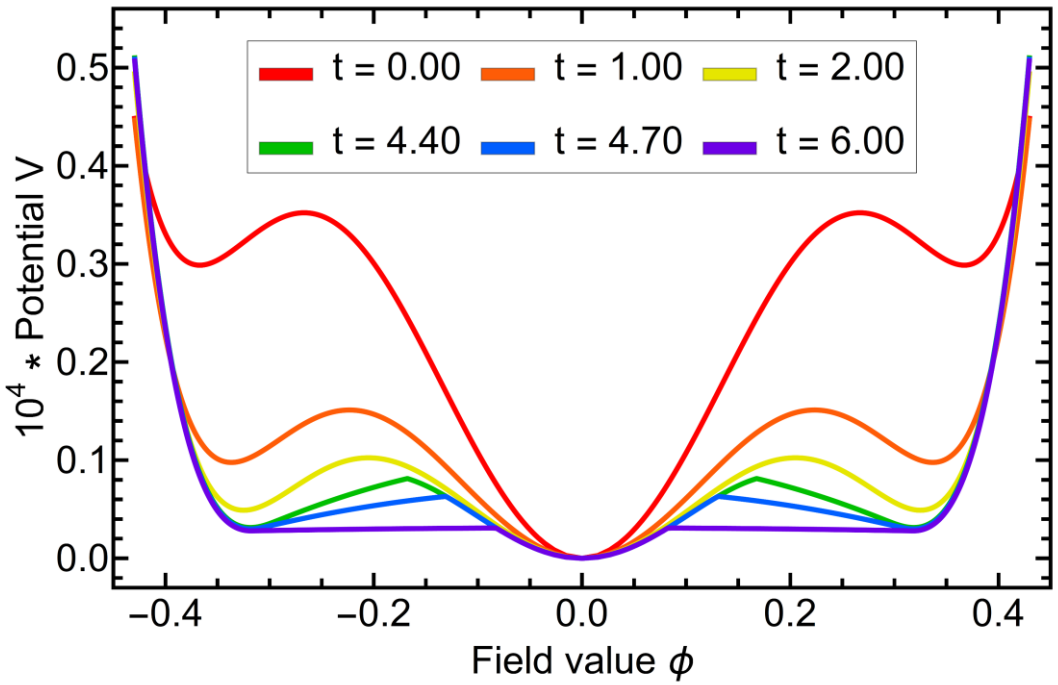
Grossi, NW, arxiv:1903.09503

Potential

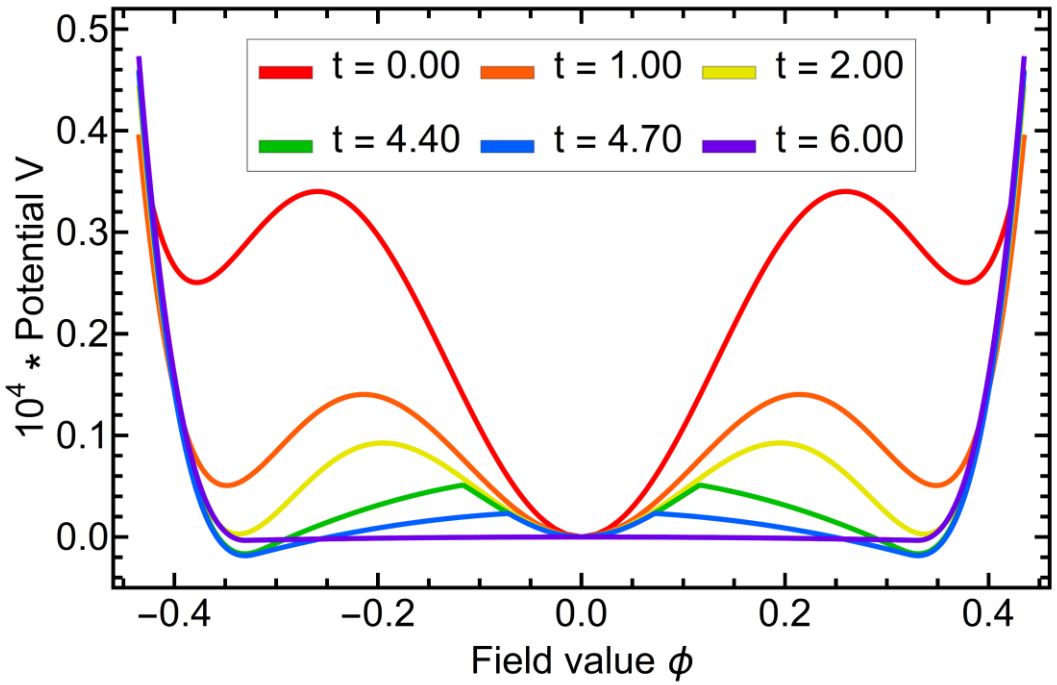
Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$

with $\lambda_4 < 0$

Symmetric phase



Broken phase



Calculated with N=5, K=200

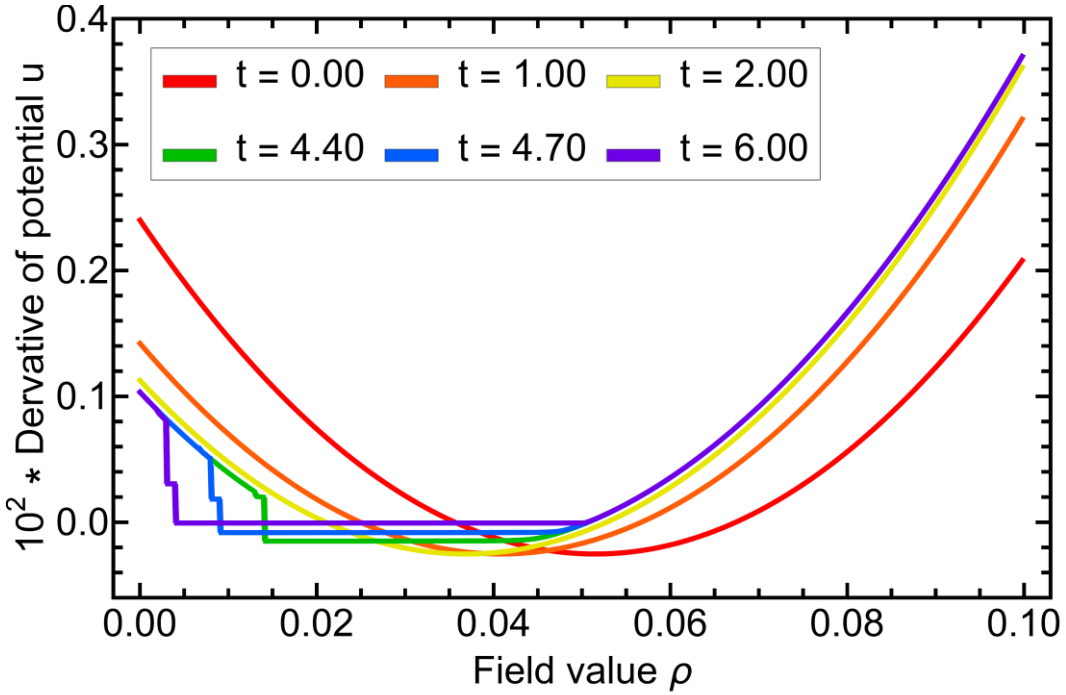
Grossi, NW, arxiv:1903.09503

Derivative

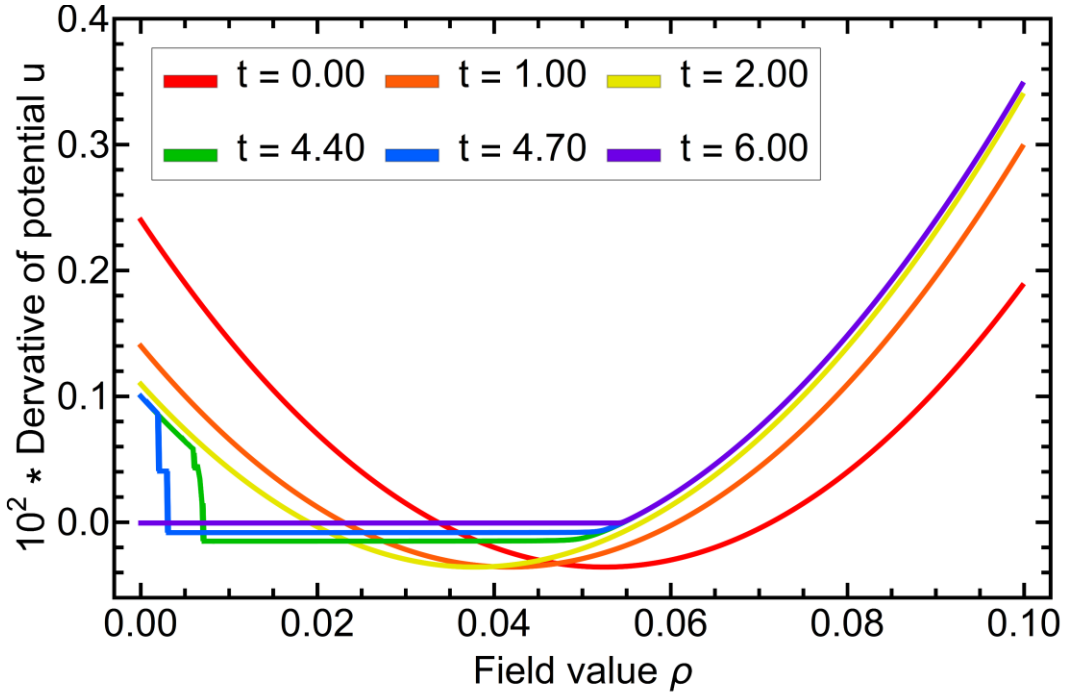
Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$

with $\lambda_4 < 0$

Symmetric phase



Broken phase



For other values of the coupling the shock doesn't freeze for positive values of the field

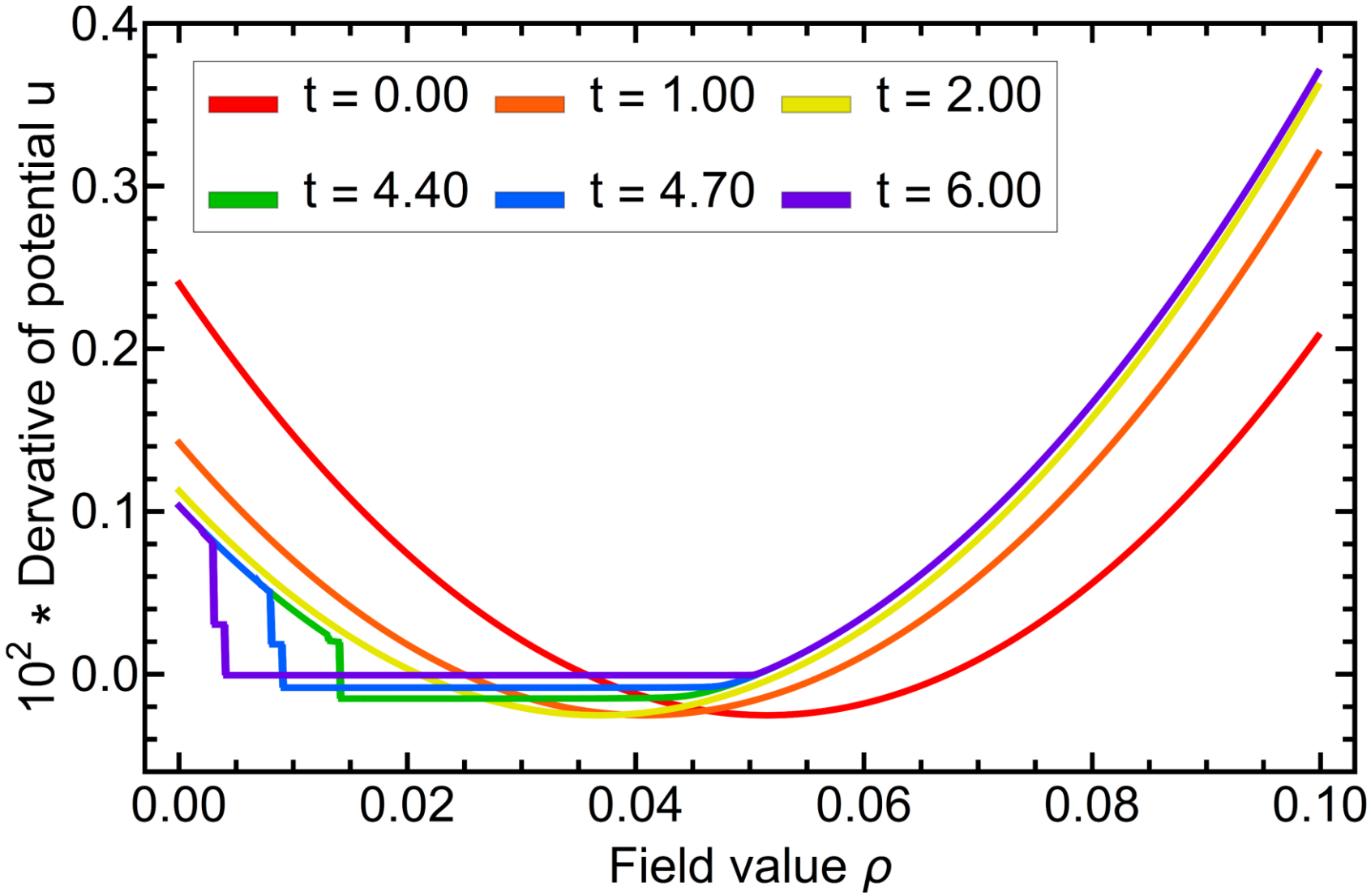
➡ Mechanism for first order phase transition in terms of shocks

Calculated with N=5, K=200

Derivative

Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$

with $\lambda_4 < 0$



- Symmetric phase
- Jump discontinuity forms and freezes in!
- Non-trivial second minimum present
- First order phase transition during the flow

Calculated with N=5, K=200

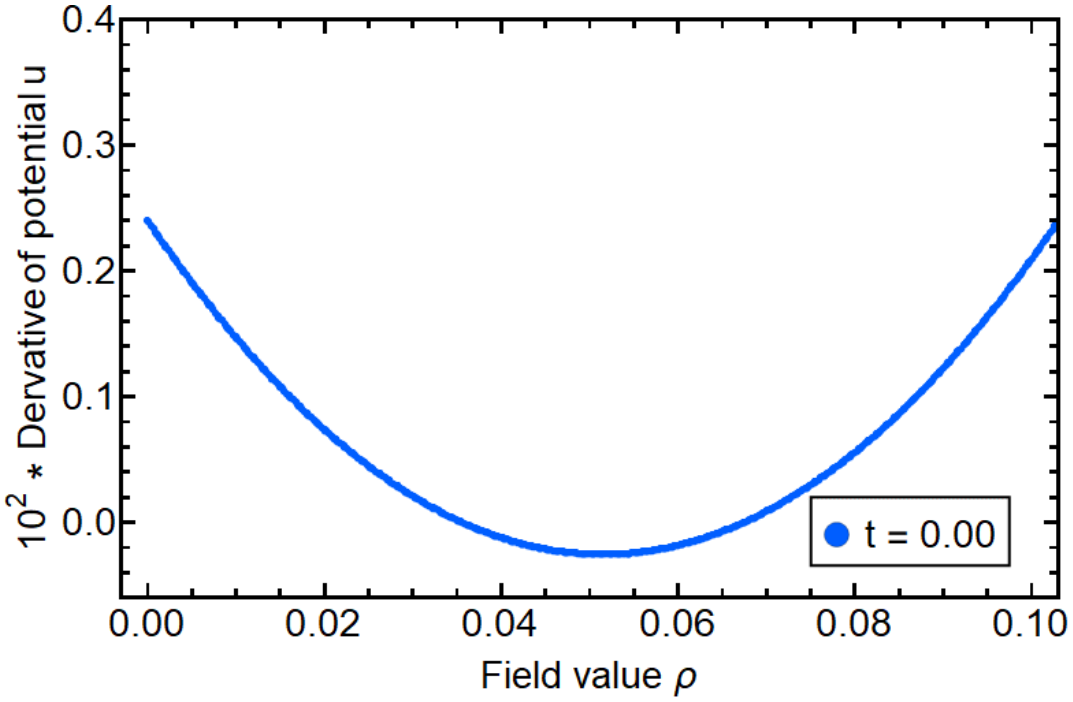
Grossi, NW, arxiv:1903.09503

Derivative

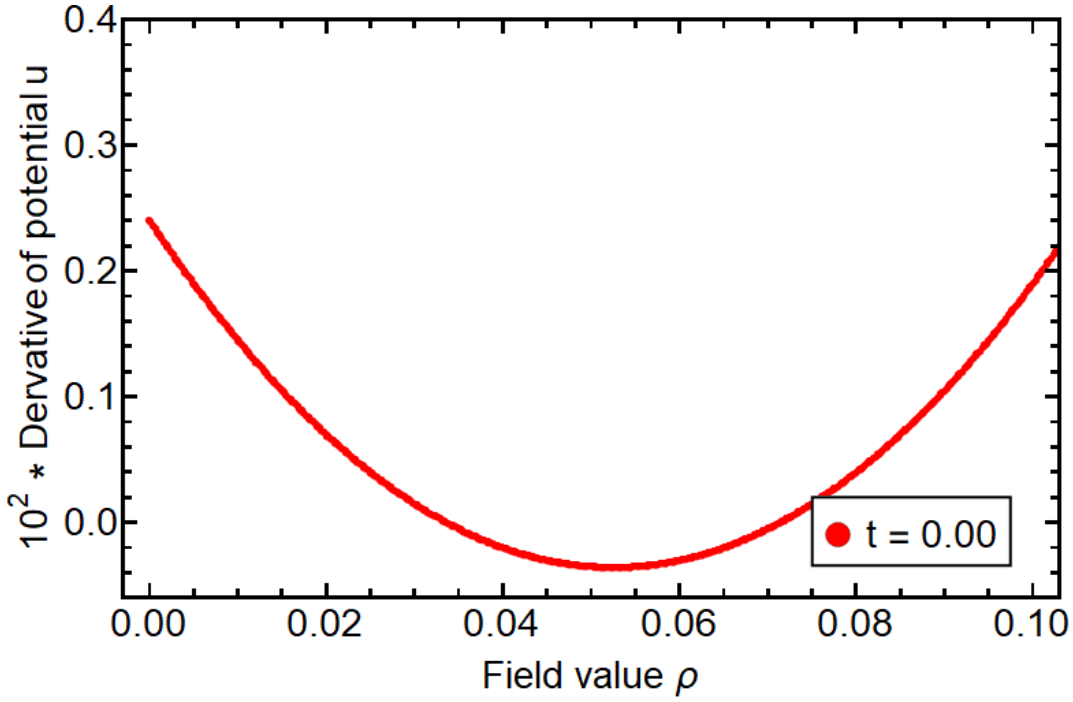
Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$

with $\lambda_4 < 0$

Symmetric phase



Broken phase



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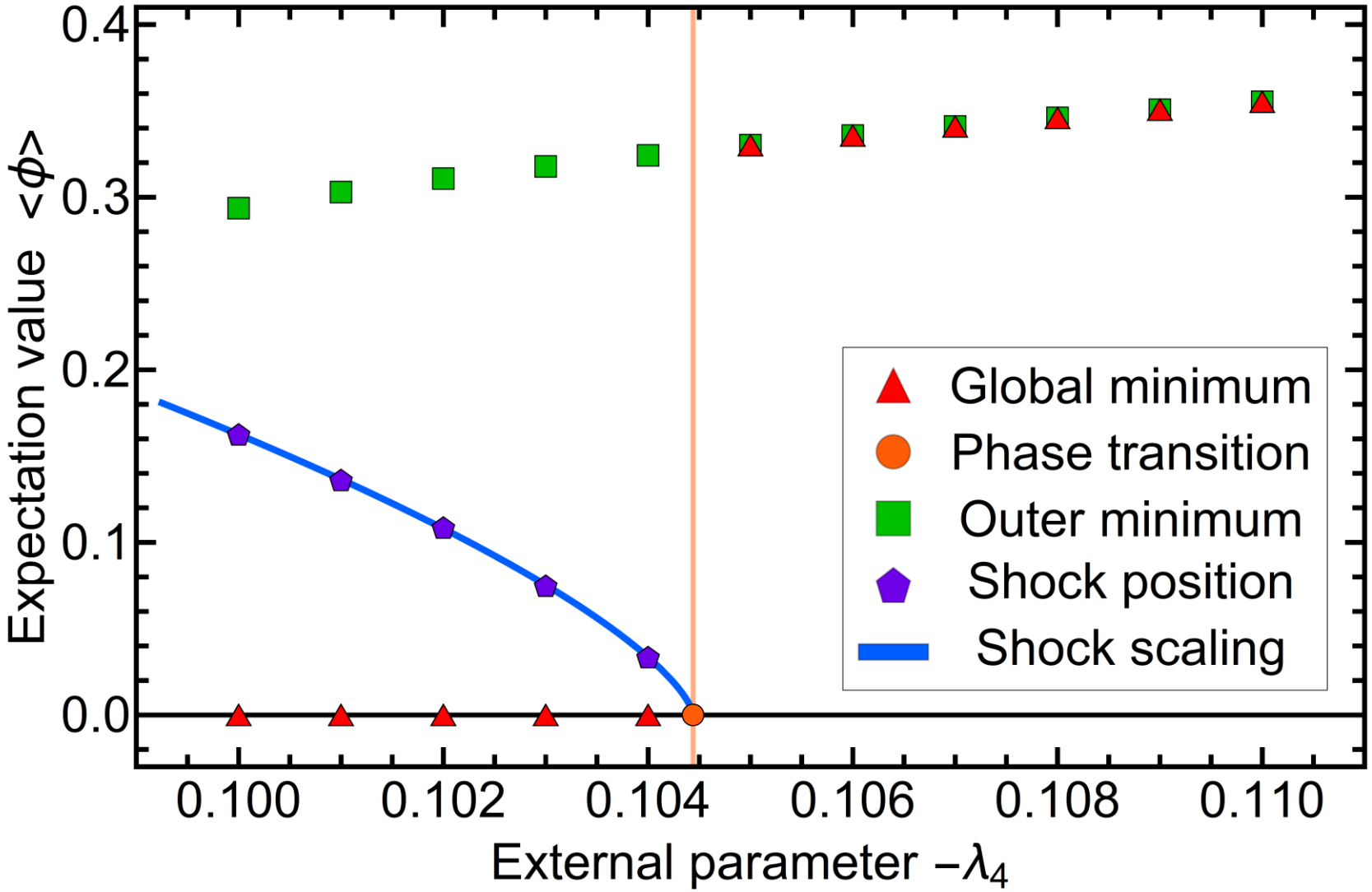
Calculated with N=5, K=200

Grossi, NW, arxiv:1903.09503

1st-order phase transition

Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$
with $\lambda_4 < 0$



- First order phase transition
- Position of the phase transition determined by "second order transition" of the position of the shock
- Shock agrees with power law (exponent: 0.68±0.01)
- Universal properties?

Calculated with N=5, K=200

Grossi, NW, arxiv:1903.09503

Beyond Large N

Including Diffusion

$$\partial_t u \;+\; \partial_x f^{(c)}(u,t,x) \;+\; \partial_x f^{(D)}(u,\partial_x u,t,x) \;=\; s(u,t,x)$$

- Reformulate as first order system

$$\partial_t u + \partial_x f(u,q) = 0$$
$$q = \partial_x u$$

- Diffusion term almost everywhere convection dominated

- Consider Finite Difference for now
  (We also did DG methods)

- Convection dominated → Upwind scheme

$$\partial_t u + D^1_{\mathrm{R}} f(u,q) = 0$$
$$q = D^1_{\mathrm{L}} u$$

Grossi, Pawlowski, NW, in prep.

Quark Meson model

Chiral phase diagram

- Quark-Meson model topic in several talks

d=4 & N=4

c.f. Talks by Carl Zelle, Fabian Rennecke, Martin Steil, ...

- Resulting phase structure well known

Braun, Pawlowski, Rennecke, Schaefer, Wambach, and many more ....

$$\partial_t u \;+\; \partial_x f^{(c)}(u,t,x) \;+\; \partial_x f^{(D)}(u,\partial_x u,t,x) \;=\; s(u,t,x)$$

Conservation term (Pions) | Diffusion term (Sigma meson) | Source term (Quarks)

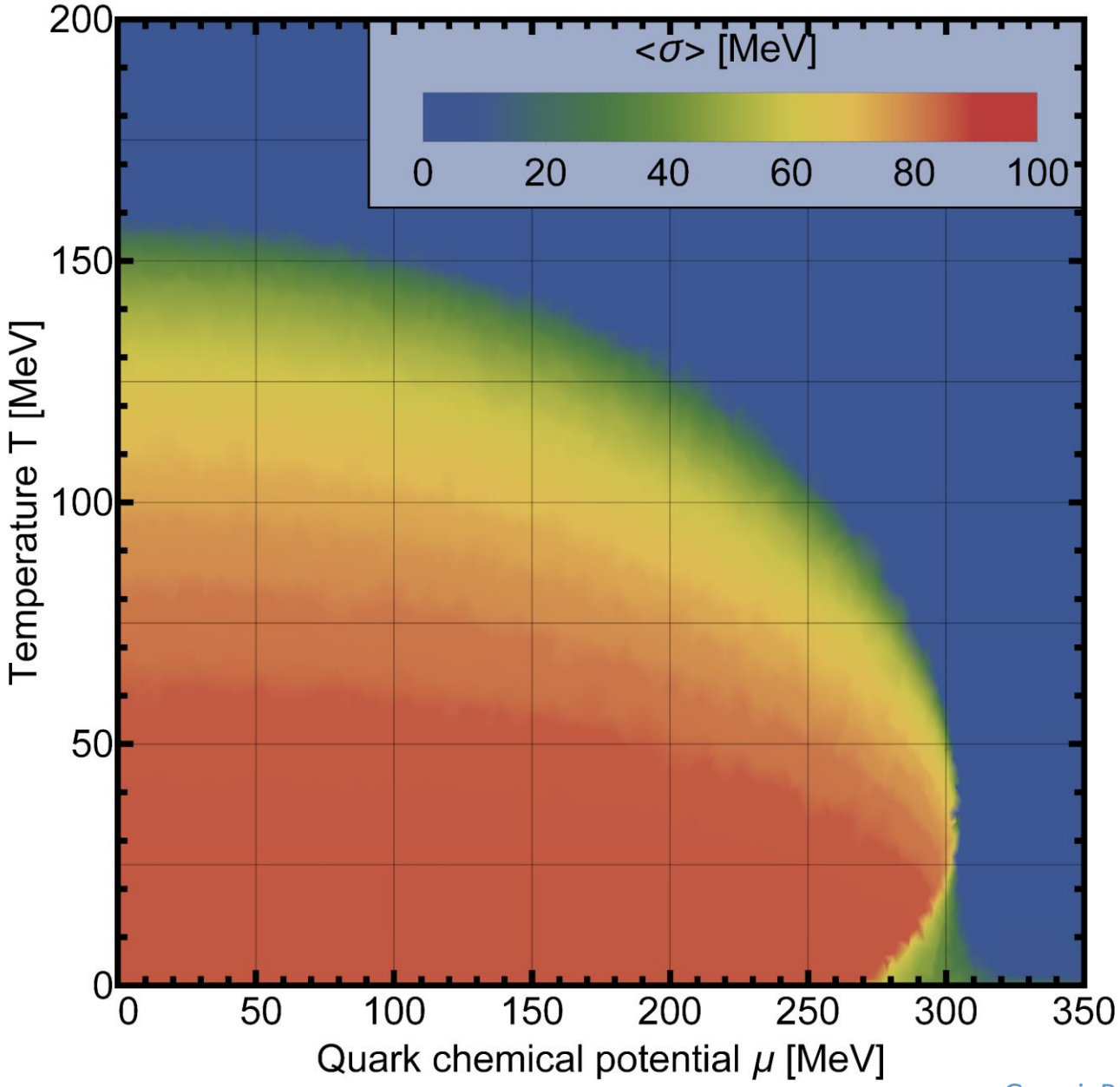
Grossi, Pawlowski, NW, in prep.

Chiral phase diagram

Stable scheme

No adjustment of grid points, final RG-time ....

Pick once and enjoy the result



Grossi, Pawlowski, NW, in prep.

DG vs FDM

$$\partial_t u + D^1_{\mathrm{R}} f(u,q) = 0$$
$$q = D^1_{\mathrm{L}} u$$

Pro & Cons of Finite Difference Methods:

- Stable
- Intuitive
- Extremely fast/easy to implement and use

- First order accurate (Godunov's theorem)
- Generalisation to higher dimensions induces headaches
- Efficient use of implicit methods becomes complicated
- Geometric flexibilty (use RG properties)
- Finite accurarcy quickly problematic (double precision)

Grossi, Pawlowski, NW, in prep.

Summary & Outlook

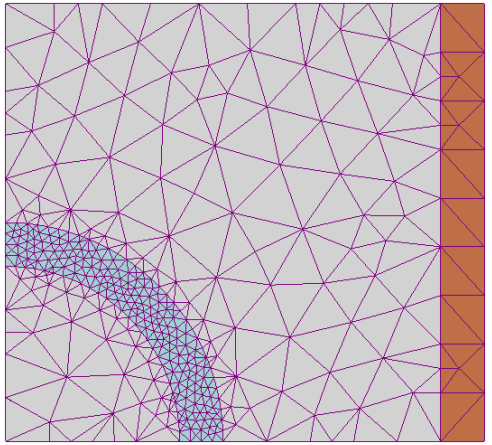
- Analogy between hydro and flow equations
- Applying Discontinuous Galerkin methods to the FRG
- Mechanism for first order phase transitions
- Robust numerical treatment in the vicinity of phase transitions

Thank you for your attention!

Discontinuous Galerkin methods

Different formulations

$$u_h^k(t,x) = \underbrace{\sum_{n=1}^{N+1} \hat{u}_n^k(t)\psi_n(x)}_{\text{Modal expansion}} = \underbrace{\sum_{i=1}^{N+1} u_h^k(t,x_i^k) l_i^k(x)}_{\text{Nodal expansion}}$$



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$$\int_{D^k} \left(\partial_t u_h^k + \partial_x f_h^k(u_h^k)\right)\psi_n \, \mathrm{d}x = 0$$

Discontinuous elements:
More degrees of freedom than equations!

Partial integration

$$\int_{D^k} \left(\left(\partial_t u_h^k\right) \psi_n - f_h^k(u_h^k)\partial_x \psi_n \right) \mathrm{d}x = -\int_{\partial D^k} \hat{\mathbf{n}} \cdot f^* \psi_n \, \mathrm{d}x$$

Weak form

Outward pointing normal vector

Numerical flux → Connects elements (closes set of equations)

Partial integration

$$\int_{D^k} \left(\partial_t u_h^k + \partial_x f_h^k(u_h^k)\right)\psi_n \, \mathrm{d}x = \int_{\partial D^k} \hat{\mathbf{n}} \cdot \left(f_h^k(u_h^k) - f^*\right) \psi_n \, \mathrm{d}x$$

Strong form

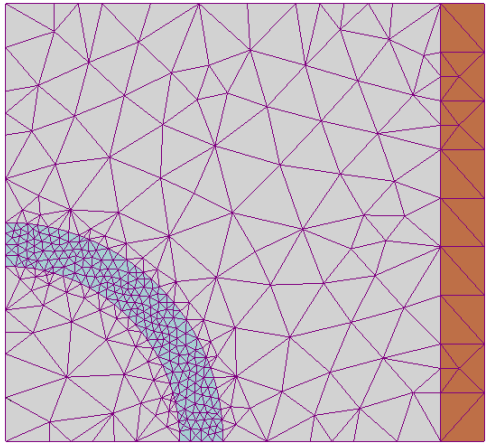
<u>Mathematically equivalent, but not numerically!</u>

Hesthaven, Warburton, Nodal Discontinuous Galerkin Methods (2008)

Implementation

Local approx

$$u_h^k(t,x) = \underbrace{\sum_{n=1}^{N+1} \hat{u}_n^k(t)\psi_n(x)}_{\text{Modal expansion}} = \underbrace{\sum_{i=1}^{N+1} u_h^k(t,x_i^k) l_i^k(x)}_{\text{Nodal expansion}}$$



Copyright: https://en.wikipedia.org/wiki/Finite_element_method

Strong form

$$\int_{D^k} \left(\partial_t u_h^k + \partial_x f_h^k(u_h^k)\right)\psi_n \,\mathrm{d}x = \int_{\partial D^k} \hat{\mathbf{n}} \cdot \left(f_h^k(u_h^k) - f^*\right)\psi_n \,\mathrm{d}x$$

Introduce matrices:

Mass matrix

$$\mathcal{M}_{ij}^k = \int_{D^k} l_i^k(x) l_j^k(x) \,\mathrm{d}x$$

Stiffness matrix

$$\mathcal{S}_{ij}^k = \int_{D^k} l_i^k(x) \partial_x l_j^k(x) \,\mathrm{d}x$$

Discretized equation

$$\mathcal{M}^k \partial_t u_h^k + \mathcal{S}^k f_h^k = \left[l^k(x)(f_h^k - f^*)\right]_{x_l^k}^{x_r^k}$$

- Only requires <u>local</u> inversion of the mass matrix
- Introducing a reference element everything is rescaled to a <u>matrix product (N x N)*(N x K)</u>

Hesthaven, Warburton, Nodal Discontinuous Galerkin Methods (2008)

Burgers equation

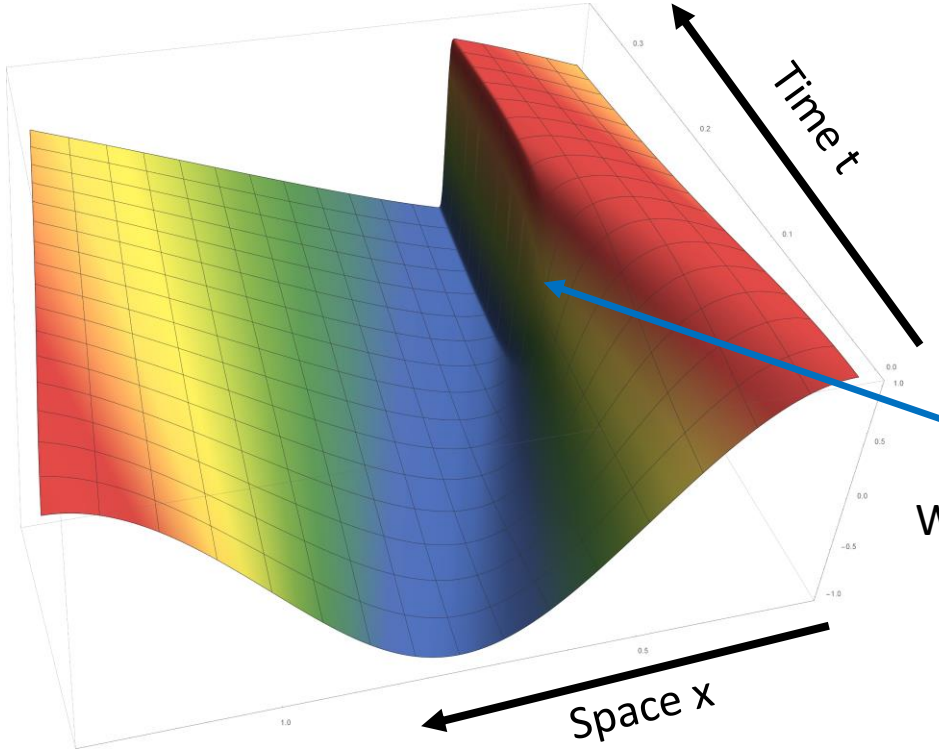
Burgers equation

$$\partial_t u + \partial_x f(u) = 0 \quad \text{with} \quad f(u) = \frac{1}{2}u^2$$

Prototype for conservation law that can develop <u>shock waves</u>

Appears in many areas of applied mathematics:

- Fluid mechanics
- Nonlinear acoustics
- Gas dynamics
- Traffic flow
- ....



- Simple wave as initial condition
- Wave breaks when characteristics meet
- Discontinuous regime well understood due to analytic solution of the viscous Burgers equation

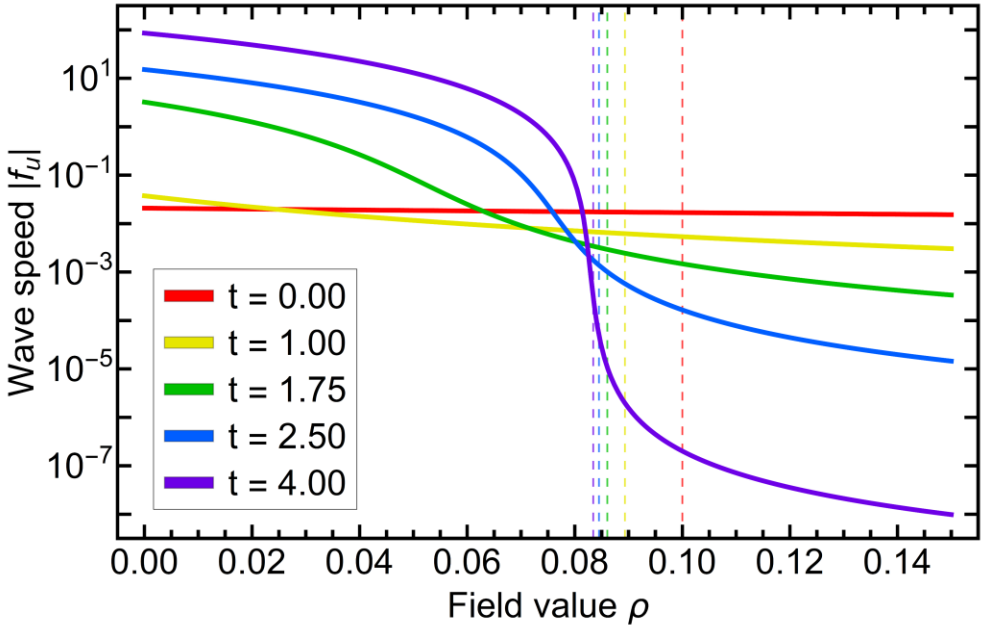
Wave breaks & shock wave forms

Second order phase transition

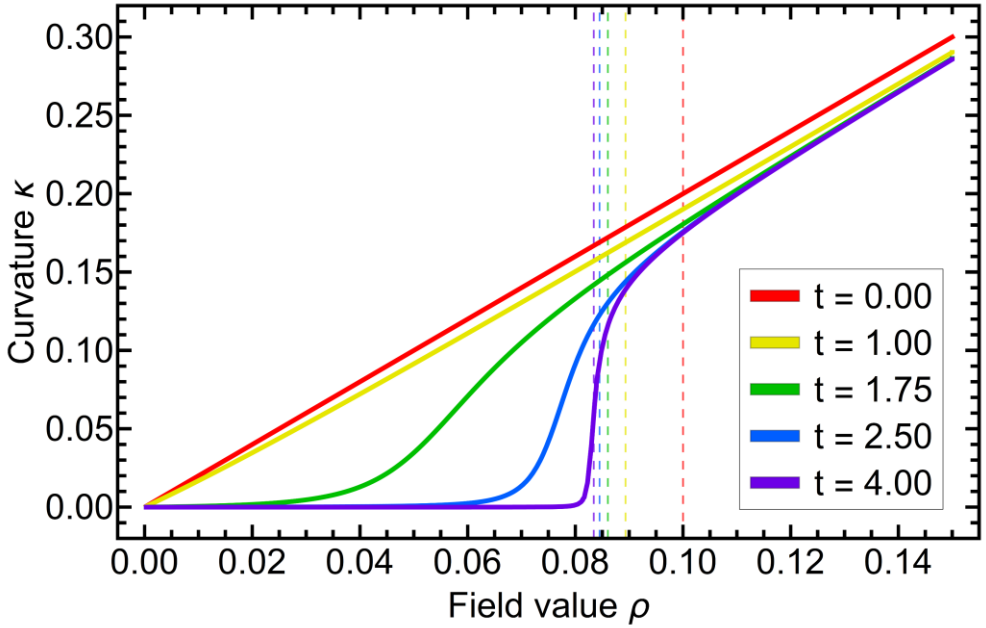
Other properties

Initial condition: $u(t=0) = -\frac{1}{10} + \rho$

Wave speed



Curvature



Wave speed strongly suppressed at large field values

Justifies Taylor methods in that regime
(only local structure relevant)

Derivatives are easily available

Riemann problem

Riemann problem

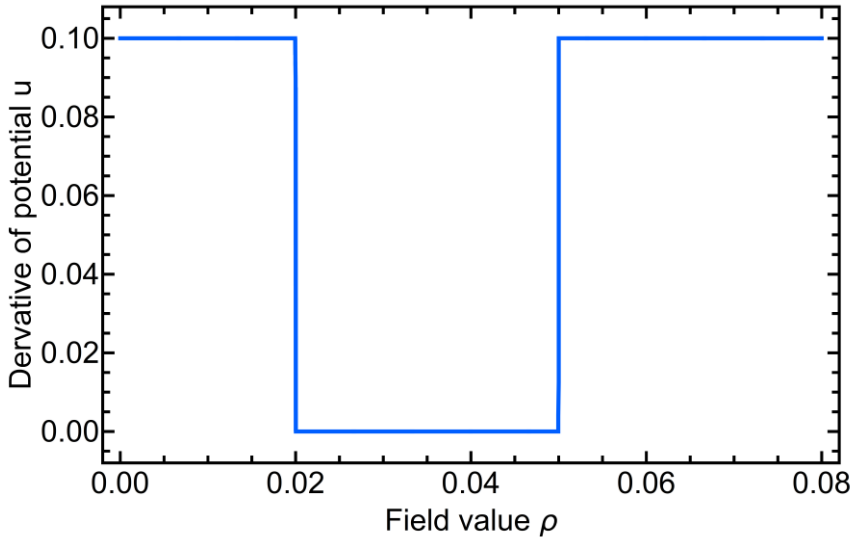
$$f(t,u) = -\frac{\Omega_d}{d(2\pi)^d}\frac{(\Lambda e^{-t})^{d+2}}{(\Lambda e^{-t})^2 + u}$$

Information flows from large to small field values and is faster for smaller values of the derivative!
What does this imply for discontinuities?

- Jump discontinuities can form if the derivative of the initial potential has a minimum
  - Relevant in physical cases

$$u(t=0) = \lambda_2 + \lambda_4\rho + \lambda_6\rho^2$$

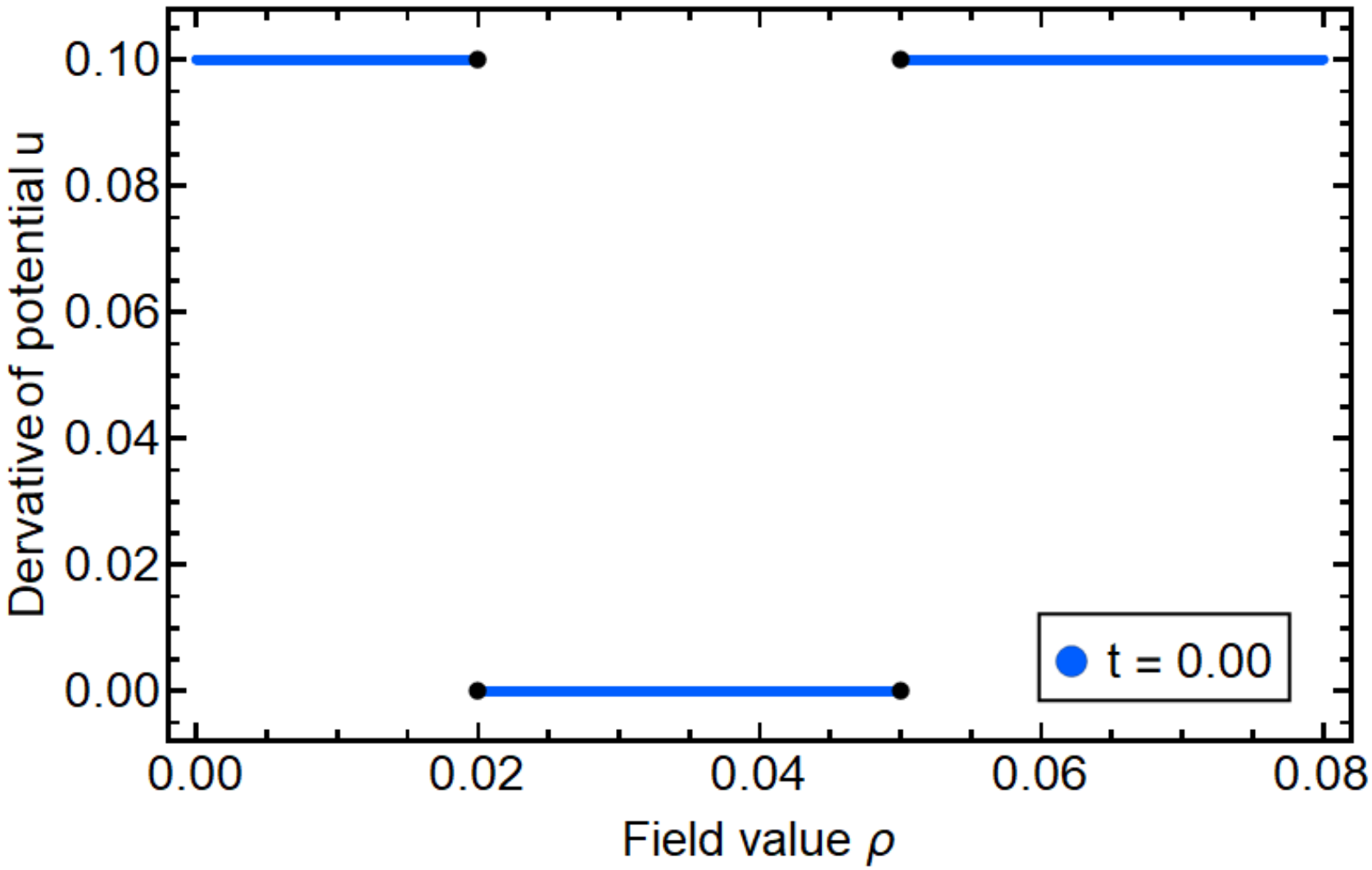
Consider the initial conditions:



Solving for piecewise constant initial conditions known as Riemann problem

- Left jump will lead to shock wave
  (Speed given by Rankine-Hugoniot condition)
- Right jump will lead to rarefaction wave
- Unique solution defined via entropy condition

Derivative

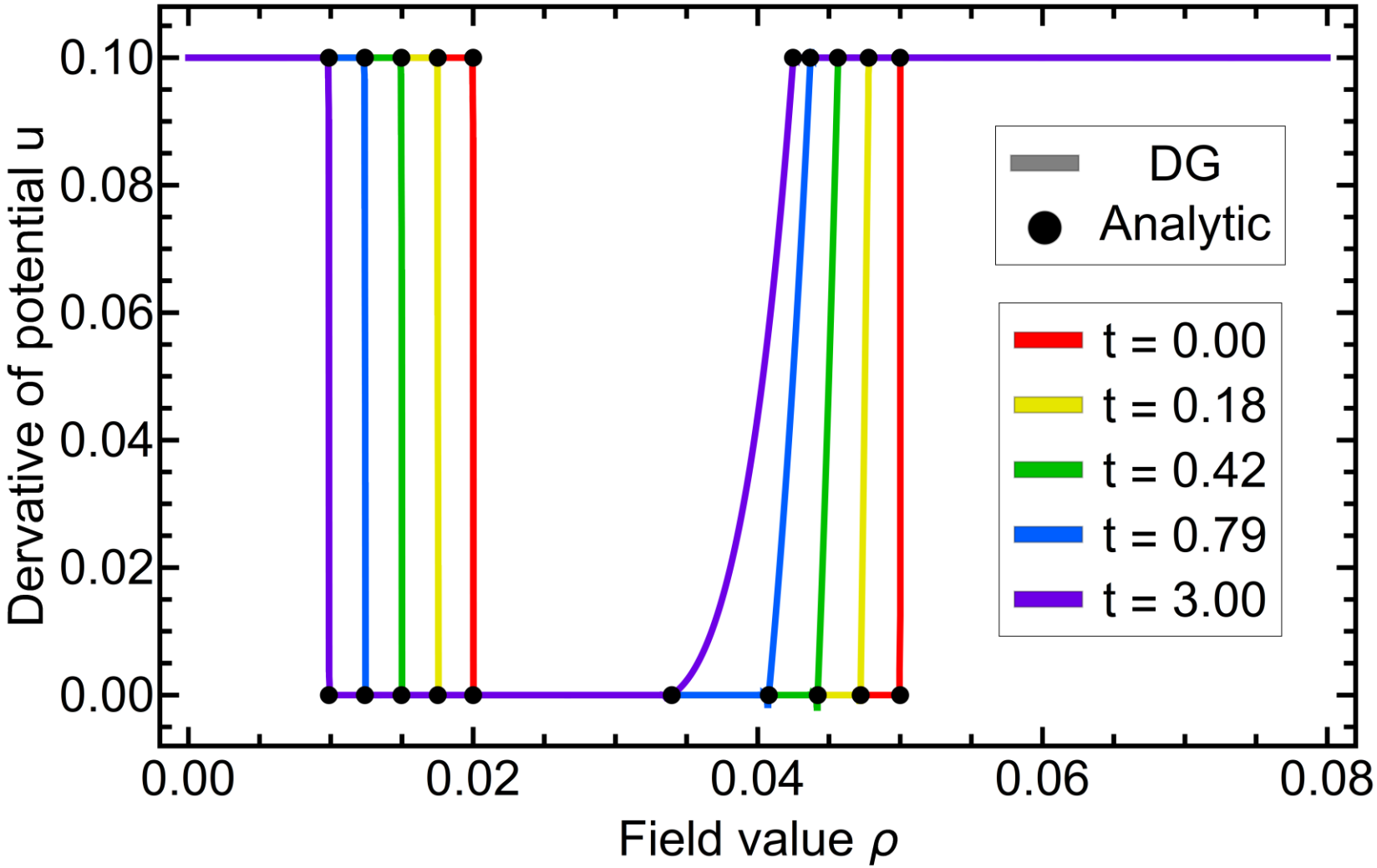


Calculated with N=3, K=1500

Derivative

Position of jump discontinuity:

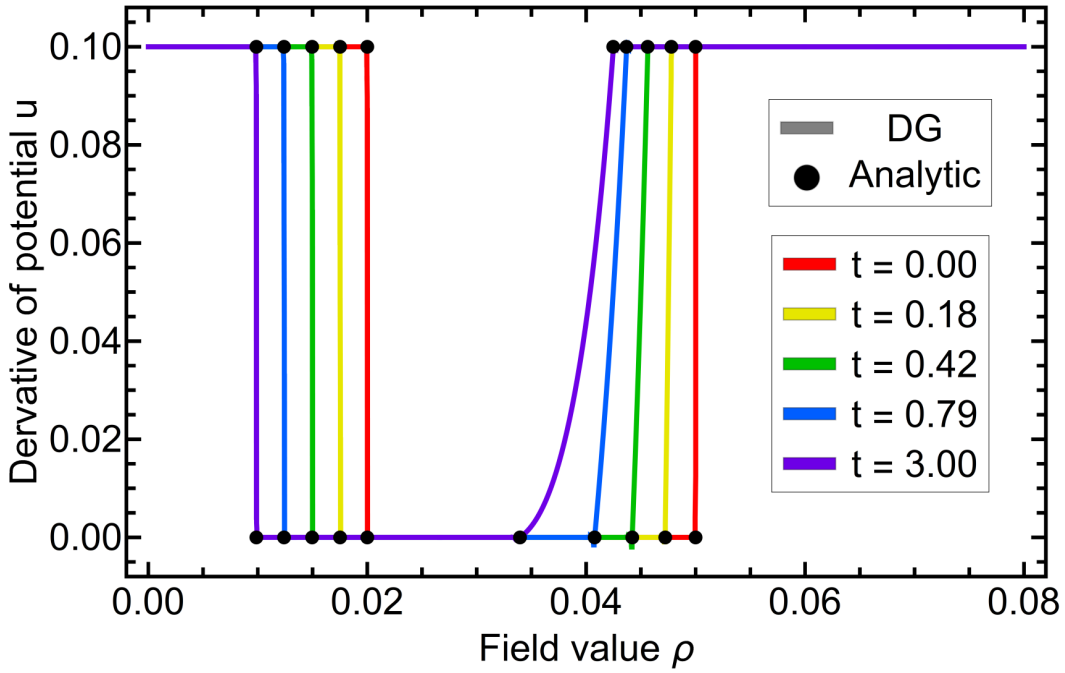
$$\xi(t) = \frac{6\pi^2\xi_0 + \sqrt{u^+}\left(\tan^{-1}\left(\frac{1}{\sqrt{u^+}}\right) - \tan^{-1}\left(\frac{e^{-t}}{\sqrt{u^+}}\right)\right) + e^{-t} - 1}{6\pi^2}$$



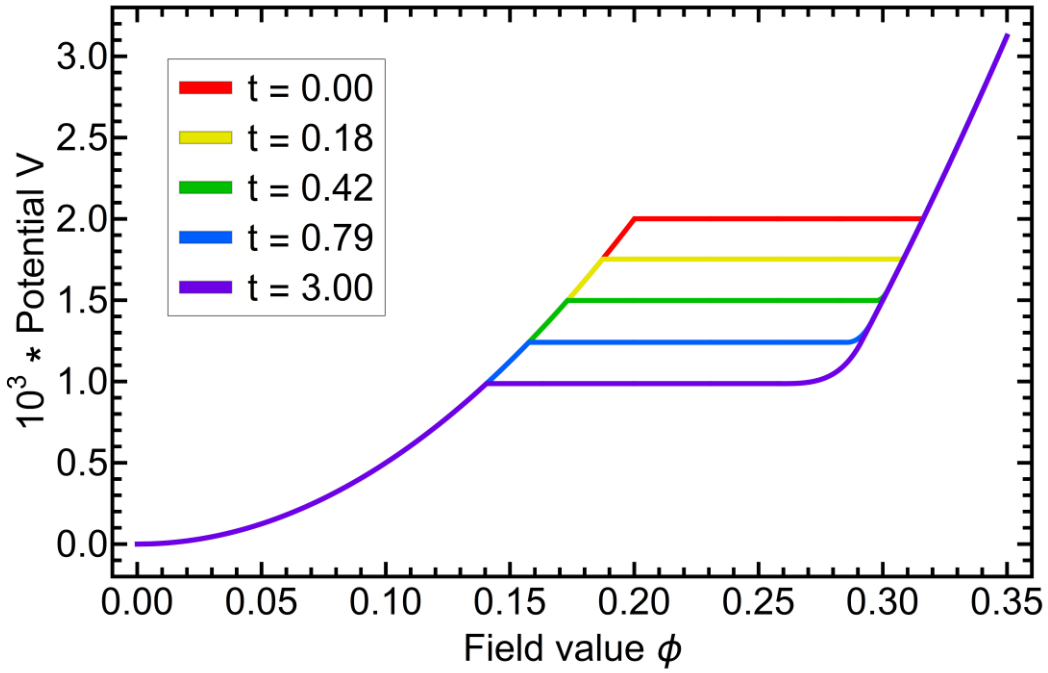
- Points of non-analyticities easily obtained analytically
- Change suppressed exponentially for large times
- Change additionally suppressed for larger jumps
- Oscillations removed in post-processing (formal accuracy can be kept!)

Calculated with N=3, K=1500

Riemann problem

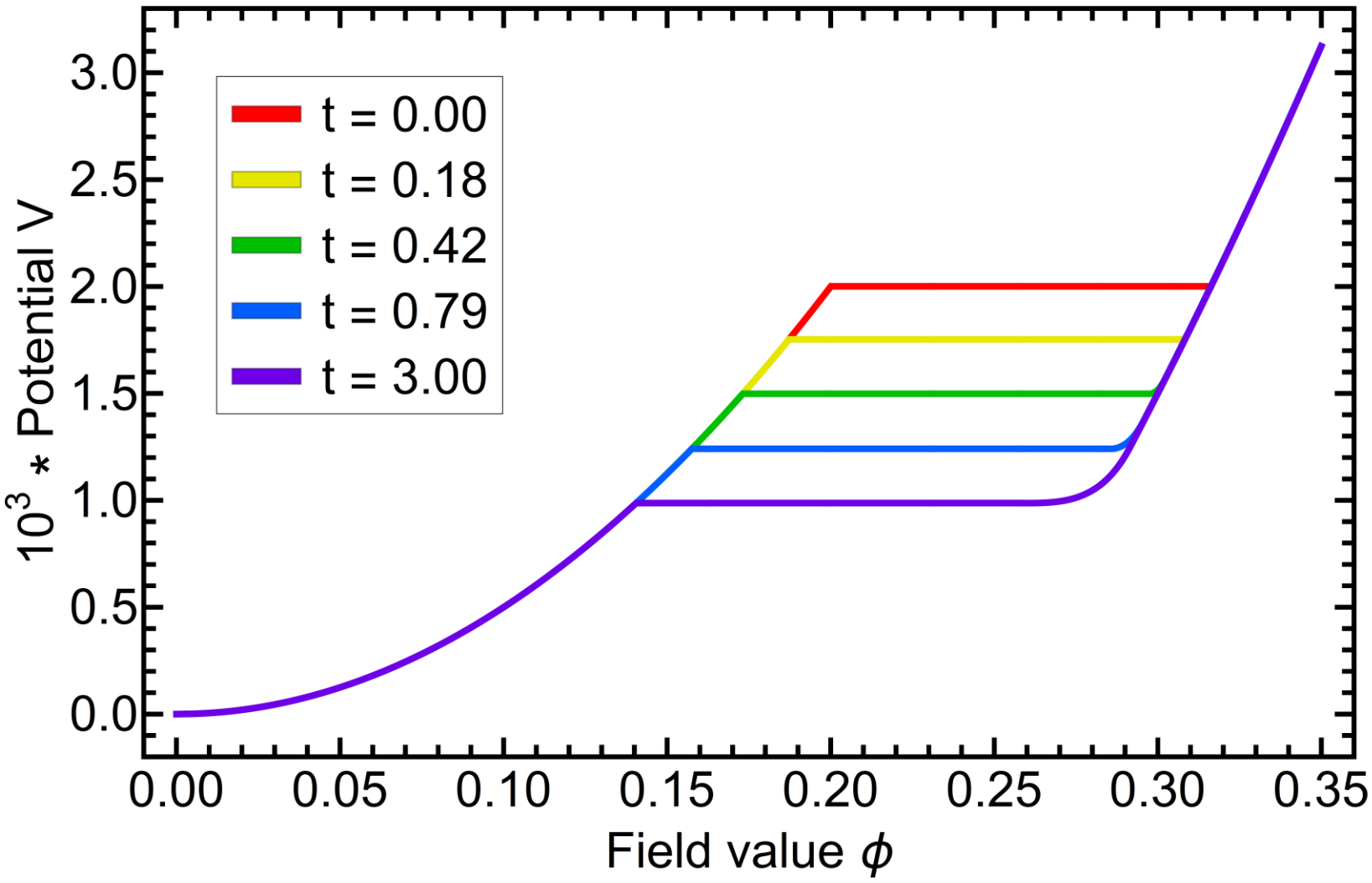


Integration



Calculated with N=3, K=1500

Potential



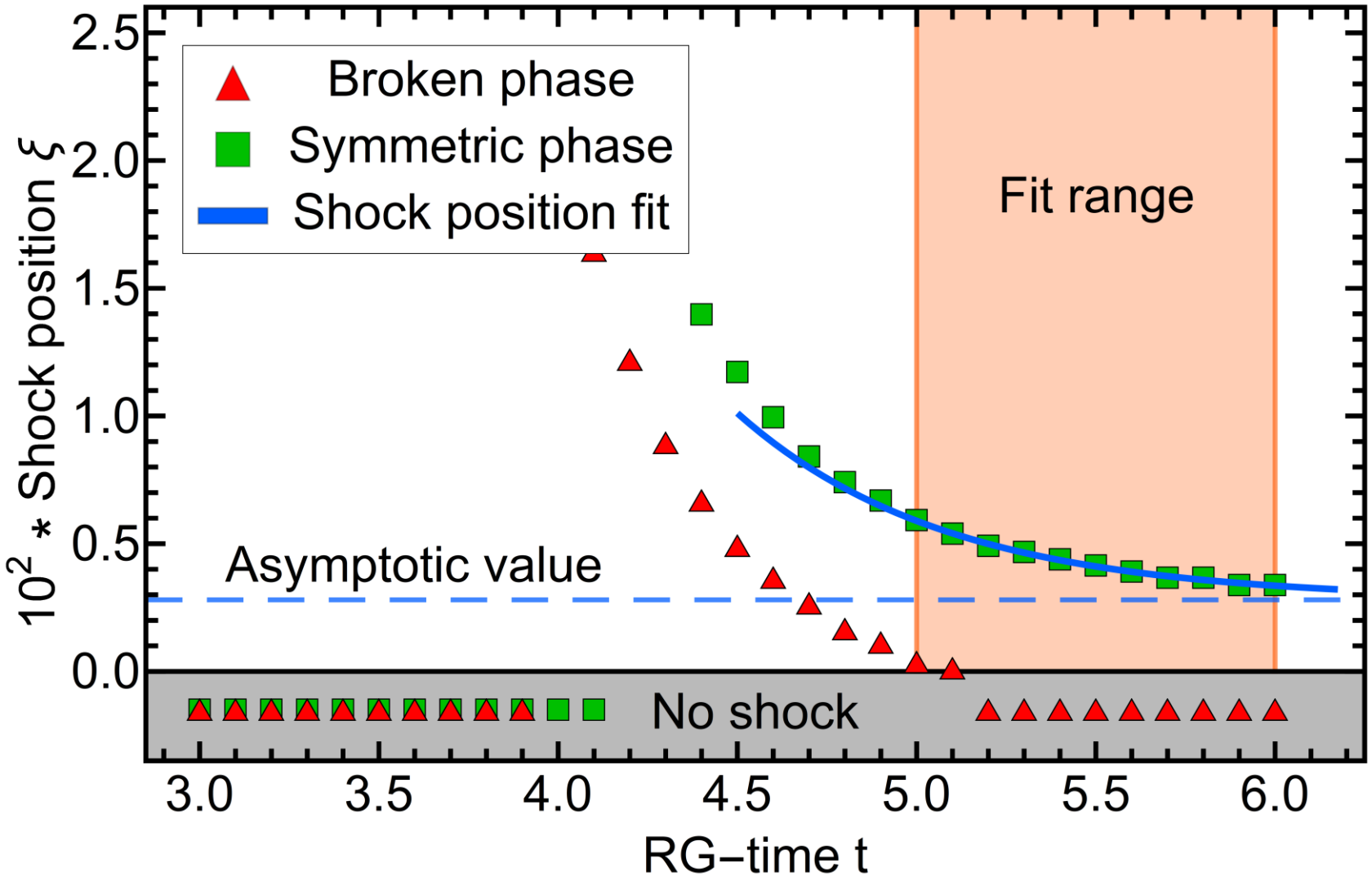
Calculated with N=3, K=1500

First order phase transition

Shock position

Initial condition: $u(t=0) = \lambda_2 + \lambda_4 \rho + \lambda_6 \rho^2$

with $\lambda_4 < 0$



- Position extracted via concentration kernel
- Asymptotic behavior determined by Riemann problem
  - ➡ Exponential decay
- Confirmed by numerical simulation
- Extrapolation to asymptotic limit easily possible

Calculated with N=5, K=200