Title: Solving initial-boundary value problems without numerical differentiation

Date: May 07, 2014 11:25 AM

URL: http://pirsa.org/14050042

Abstract: The numerical solution of nonlinear partial differential equations with nontrivial boundary conditions is central to many areas of modelling. When high accuracy is required (pseudo) spectral methods are usually the first choice. Typically in this approach we search for the pre-image under a linear operator which represents a combination of spatial derivatives along with the boundayr conditions in every time step. This operator can be quite ill-conditioned. On a basis of Chebyshev polynomials for instance the condition number increases algebraically with the number of basis functions. I will present an alternative method based on recent work by Viswanath and Tobasco which avoids numerical differentiation entirely through the use of Green's functions. I will demonstrate this method on the Kuramoto-Sivashinsky equation with fixed boundary conditions.

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Solving initial-boundary value problems without numerical differentiation

Lennaert van Veen

Outline

1. Motivation

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2. Using Green's function
3. Kuramoto-Sivashinsky

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4. Computing Green's function

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3. Kuramoto-Sivashinsky
4. Computing Green's function
5. Proper quadrature

Motivation – Setup

$u_t = Lu + f(u)$ e.g. Navier-Stokes, reaction-diffusion, ...

$$\left.\begin{array}{l} u(-1) = a_0,\ u'(-1) = a_1, \dots \\ u(1) = b_0,\ u'(1) = b_1, \dots \end{array}\right\} \text{sufficiently many BC}$$

$u(x,0) = u_0(x)$ initial value

Central question: what method enables us to find solutions

- with accurately resolved boundary layers;
- that are stable to overresolution;
- that are not prohibitively expensive to compute?

Step 1: implicit-explicit time discretization, e.g.

$$\frac{u^{k+1} - u^k}{\Delta} = Lu^{k+1} + f(u^k) \quad \text{or} \quad [\mathbb{I} - \Delta L]\, u^{k+1} = u^k + \Delta f(u^k)$$

- Balances stability with computation time.
- Gives linear BVP for u^{k+1} given u^k.
- Can be exended to higher order (SBDF).
- The properties of $\mathcal{L} = \mathbb{I} - \Delta L$ are quintessential.

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Pros and cons:

- Finite differences: $u(x,t) \rightarrow \{u_j(t)\}$ where $u_j(t) \approx u(x_j,t)$.
  - Pro: $\mathcal{L}$ represented by a sparse, banded matrix so solving is fast.
  - Pro: Easy to program.
  - Con: Low accuracy – $O(h^q)$ for fixed q.
  - Con: Not stable to overresolution.

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- Pseudo spectral method: $u(x,t) \rightarrow \{a_k\}$ where $u(x,t) \approx \sum_k a_k(t) T_k(x)$.
  - Pro: High accuracy – "$q = \infty$".
  - Con: $\mathcal{L}$ represented by dense matrix.
  - Con: BC are *global* conditions on the variables.
  - Pro: For Chebyshev basis, $O(n \ln n)$ methods for computing $\mathcal{L}v$ available.
  - Con: Condition number of $\mathcal{L}$ + BC grows algebraically, e.g. $O(n^{2p})$ for Chebysev.

Green's function – *invert first*

Both ideas are based on *discretizing first, then inverting*. With Green's function, we can *invert exactly, then discretize*:

$$u^{(k+1)} = \int_{y=-1}^{1} G(x,y)\left(u^k(y) + \Delta f(u^k(y))\right) \mathrm{d}y$$

where $G \in C^{p-2}$ satisfies

$$\mathcal{L}G(x,y) = \Delta(x-y)$$

The RHS now requires *numerical integration* instead of *differentiation*, which is much more stable.
The question is: what quadrature to use?

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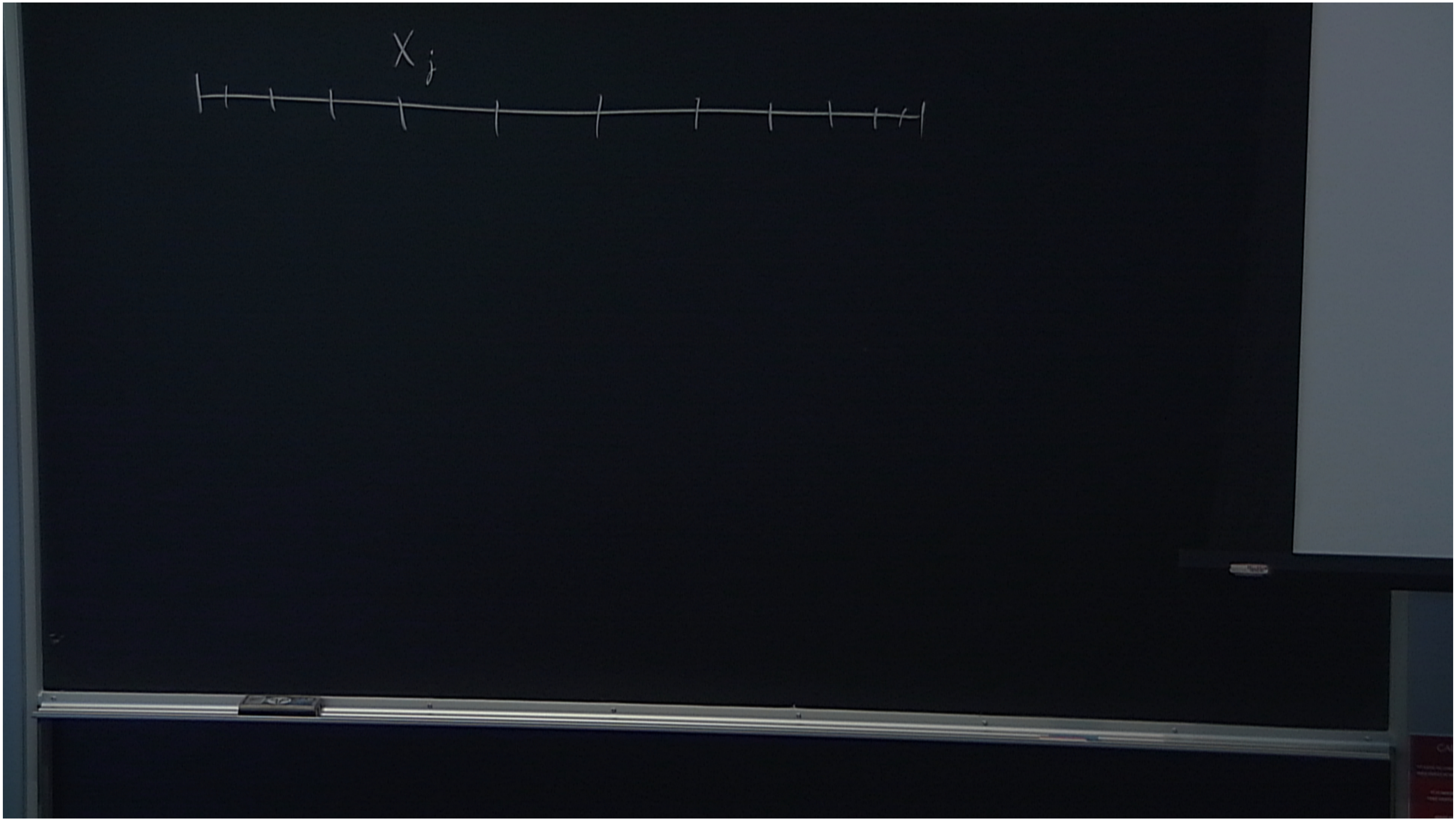
Summarising:

For Chebyshev pseudospectral method (or similar):

- must either find and decompose $\mathcal{L}_\mathrm{d}$ for $\mathrm{O}(n^2)$ or use spectral differentiation to find $\mathcal{L}_\mathrm{d} v$ for $\mathrm{O}(n \ln n)$;
- fundamental limitation is the conditioning of $\mathcal{L}_\mathrm{d}$.

For Green's function based solving:

- must find a quadrature the is accurate even for the *finitely differentiable* integrand;
- fundamental limitation: ?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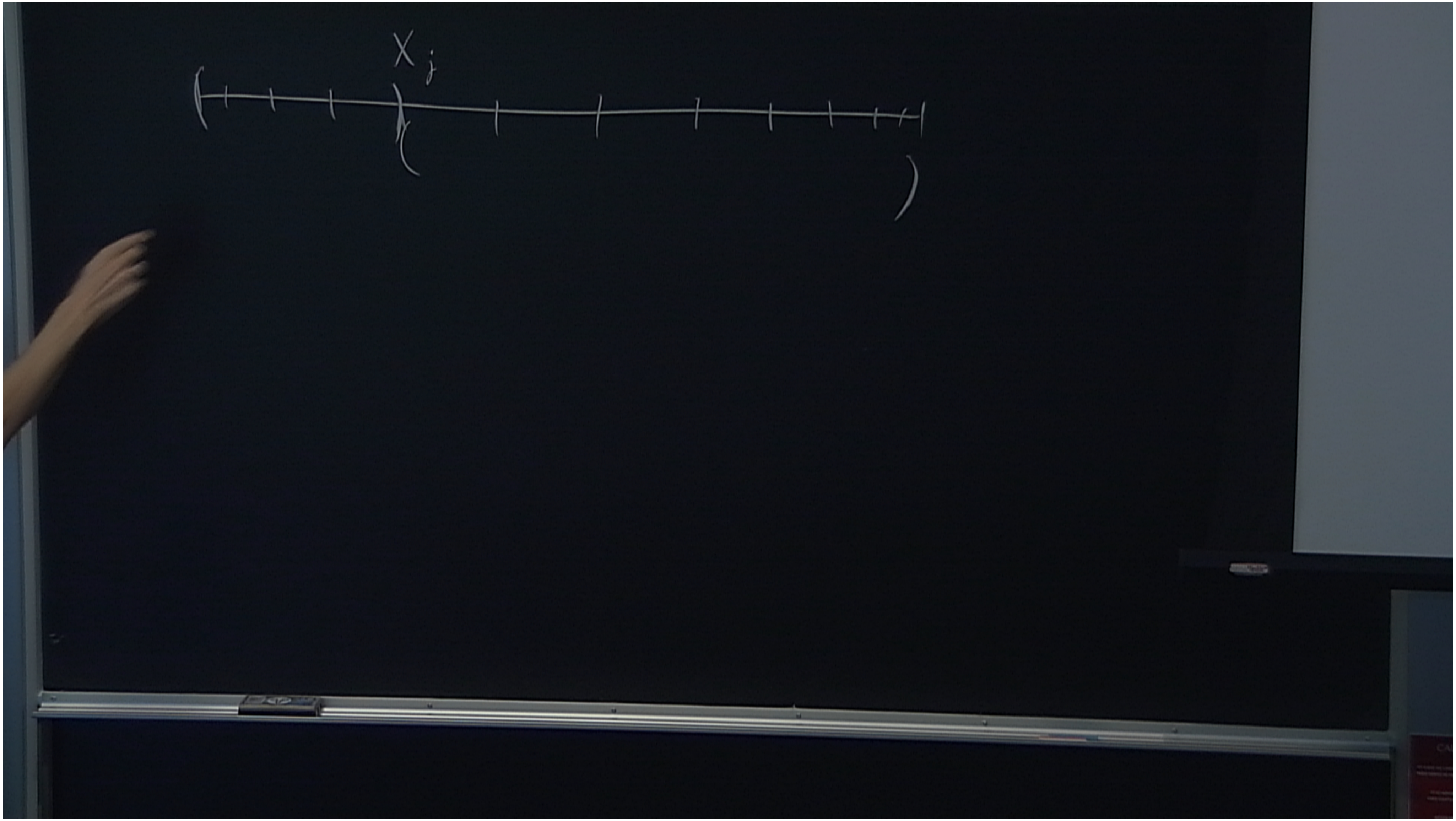
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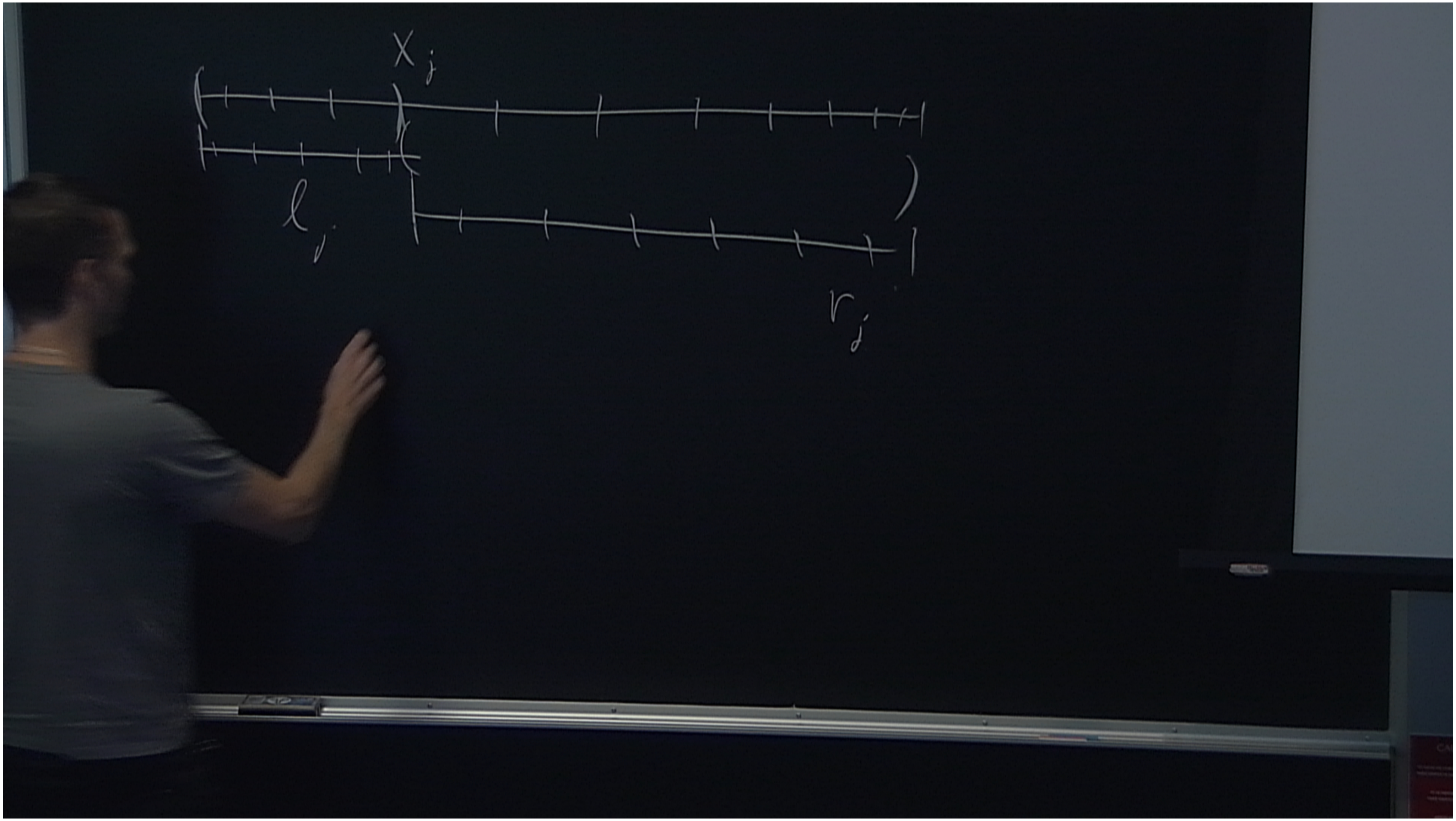
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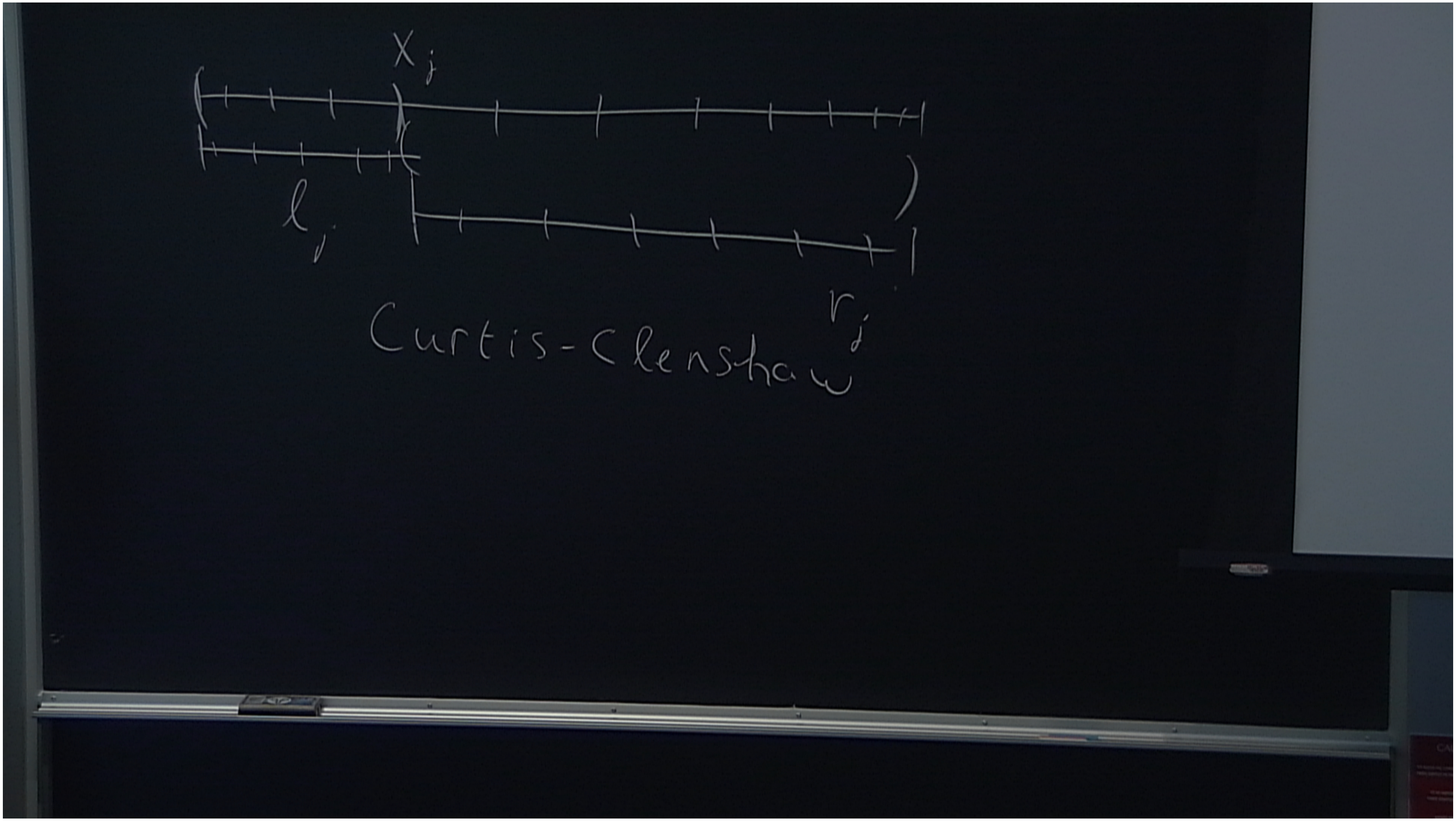
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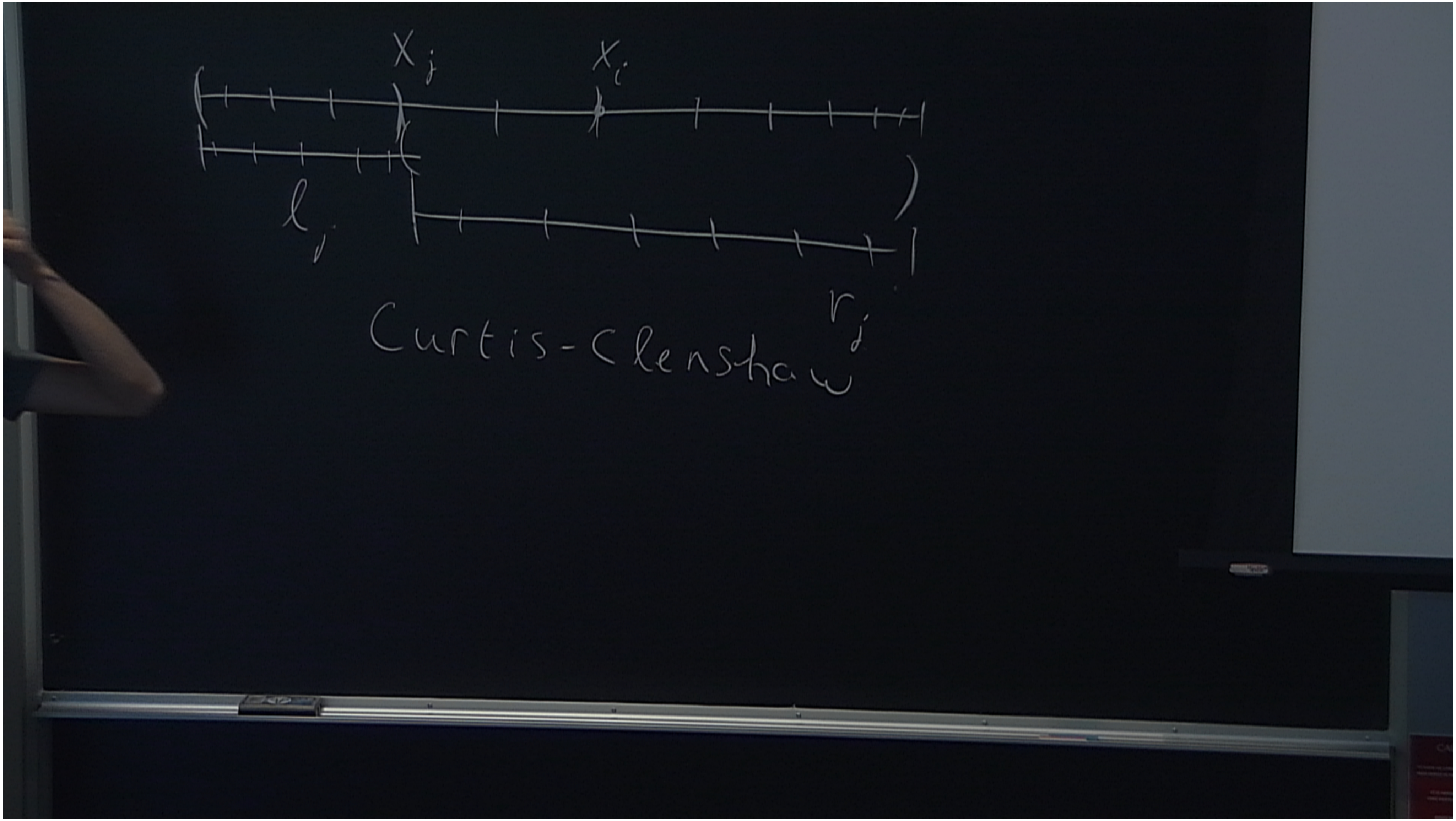
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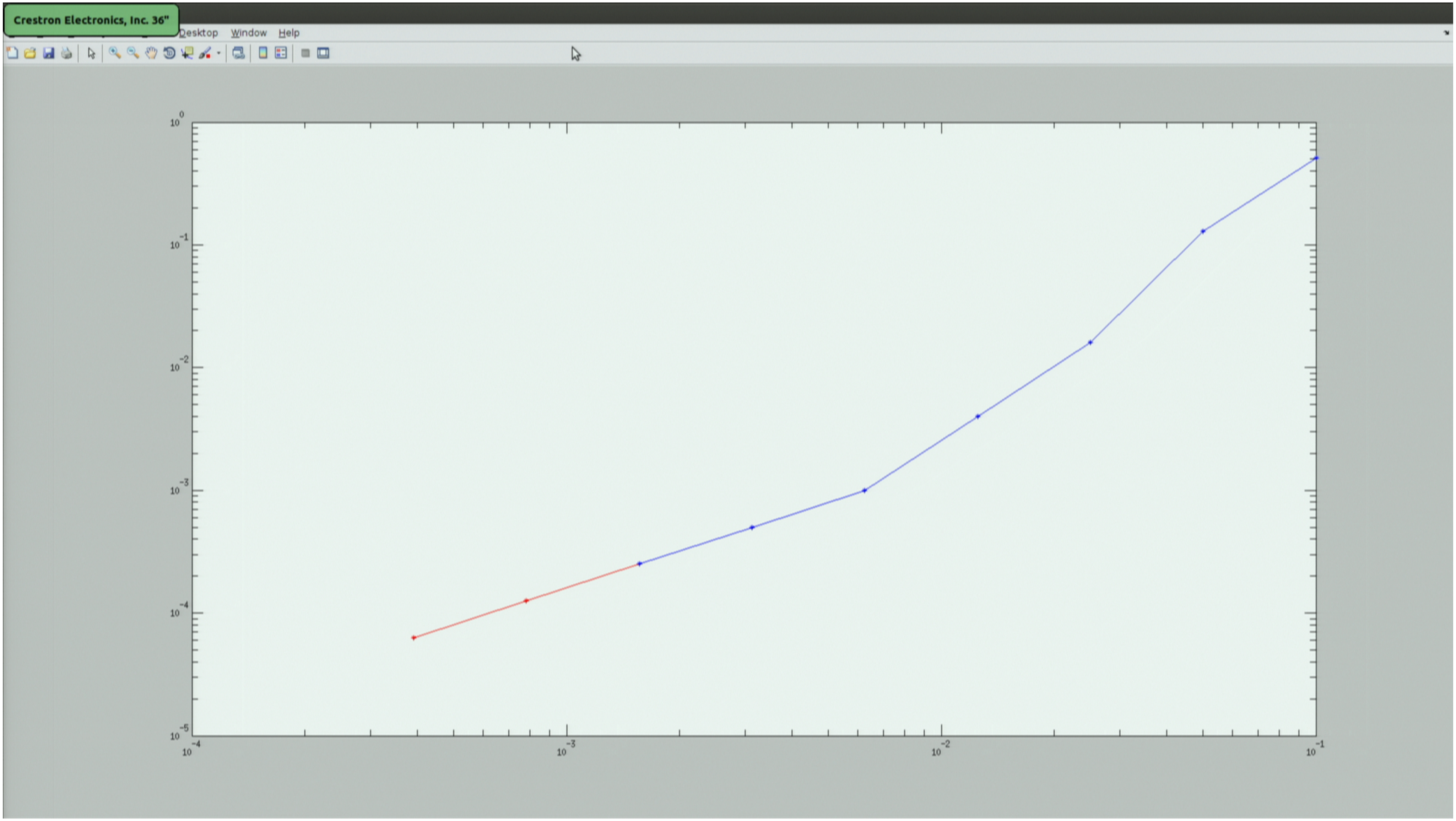
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KS equation – Kuramoto-Sivashinsky IBVP

$$
\begin{aligned}
u_t + uu_x + u_{xx} + \nu\, u_{xxxx} &= 0 \\
-u(-1,t) = u(1,t) &= R \\
u_{xx}(-1,t) = u_{xx}(1,t) &= 0 \\
u(x,0) &= u_0(x)
\end{aligned}
$$

Set $\phi = Rx$, $u = v + \phi$, then

$$
\begin{aligned}
v_t &= \left[-\partial_x^2 - \nu\partial_x^4 - R\right] v + vv_x + \phi v_x + R\phi \\
v(-1,t) = v_{xx}(-1,t) &= v(1,t) = v_{xx}(1,t) = 0
\end{aligned}
$$

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KS Green's function – computing it

The linear operator

$$\mathcal{L} = \mathbb{I} + \Delta\partial_x^2 + \Delta\nu\partial_x^4 + \Delta R$$

is *symmetric* with these BC.
Spectrum:

Odd: $w_k^{\mathrm{o}} = \sin(k\pi x)$

$$\lambda_k^{\mathrm{o}} = 1 + \Delta R - \Delta\pi^2 k^2 + \Delta\nu\pi^4 k^4$$

Even: $w_k^{\mathrm{e}} = \cos\left(\left[k - \frac{1}{2}\right]\pi x\right)$

$$\lambda_k^{\mathrm{e}} = 1 + \Delta R - \Delta\pi^2\left(k - \frac{1}{2}\right)^2 + \Delta\pi^4\nu\left(k - \frac{1}{2}\right)^4$$

Eigenfunction expansion of G:

$$G(x,y) = \sum_{k=1}^{\infty} \left\{ \frac{w_k^{\mathrm{o}}(x)\, w_k^{\mathrm{o}}(y)}{\lambda_k^{\mathrm{o}}} + \frac{w_k^{\mathrm{e}}(x)\, w_k^{\mathrm{e}}(y)}{\lambda_k^{\mathrm{e}}} \right\}$$

Odd terms:

$$\sum_{k=1}^{\infty} \frac{w_k^{\mathrm{o}}(x)\, w_k^{\mathrm{o}}(y)}{\lambda_k^{\mathrm{o}}} = \frac{1}{2\Delta\nu(z_+ - z_-)} \sum_{k=1}^{\infty} \left\{ \frac{\cos(k\pi\,[x-y])}{\pi^2 k^2 - z_+} - \frac{\cos(k\pi\,[x-y])}{\pi^2 k^2 - z_-} - \frac{\cos(k\pi\,[x+y])}{\pi^2 k^2 - z_+} + \frac{\cos(k\pi\,[x+y])}{\pi^2 k^2 - z_-} \right\}$$

where

$$z_{\pm} = \frac{1}{2\nu} \pm \frac{1}{2\Delta\nu}\sqrt{\Delta^2 - 4\Delta\nu(1+\Delta R)} \text{ solve } \lambda_k^{\mathrm{o}} = 0 \text{ with } z = \pi^2 k^2$$

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…and after some mucking around:

$$\sum_{k=1}^{\infty} \frac{w_k^{o}(x) w_k^{o}(y)}{\lambda_k^{o}} =$$

$$\Re\left(\frac{1}{4\Delta\nu(z_+ - z_-)}\left\{\check{f}_+(x-y) - \check{f}_-(x-y) - \check{f}_+(x+y) + \check{f}_-(x+y)\right\}\right)$$

using the ISFT and

$$f_\pm = \frac{1}{\pi^2 k^2 - z_\pm}; \quad \check{f}_\pm(x) = -\frac{\cos(\pi p_\pm - \pi p_\pm |x|)}{\pi p_\pm \sin(\pi p_\pm)}, \quad \pi^2 p_\pm^2 = z_\pm$$

And similar for the even terms.

Finally:

$$G(x,y) = \frac{i}{\pi\Delta\nu(z_+ - z_-)} \Im\left(\frac{-\cos(2\pi p_+ - \pi p_+|x-y|) + \cos(\pi p_+|x+y|)}{p_+\sin(2\pi p_+)}\right)$$

Remarks:

- Assume that $\Delta < 4\nu/(1-4\nu R)$ so that $z_+ = z_-^*$.
- G is rewritten before numerical evaluation.
- G is smooth away from $x = y$.
- Use integration by parts for $\int G(x,y)u(y)u_y(y)\,\mathrm{d}y$

Simple idea:

- Make one master grid $\{x_j\}$.
- For each x_j, make two subgrids to cover $[-1, x_j]$ and $[x_j, 1]$, use quadrature separately on each.

The difficulty is that the sub grids are not *nested*.