Spectral Methods and Inverse Problems

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Outline

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- Fourier Spectral Methods
 - Fourier Transforms
 - Trigonometric Polynomial Interpolants
 - FFT
 - Regularity and Fourier Spectral Accuracy
 - Wave PDE

2 System Modeling

- Direct vs. Inverse
- PDE Reconstruction
- Chebyshev Spectral Methods
 - Algebraic Polynomial Interpolation
 - Potential Theory
 - Chebyshev Spectral Derivative Matrix
 - Regularity and Chebyshev Spectral Accuracy
 - Allen-Cahn PDE



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Finite Differences

- Consider grid $\{x_1, \ldots, x_N\}$ with uniform spacing h and corresponding data values $\{u_1, \ldots, u_N\}$.
- For simplicity, assume periodicity $u_0 := u_N$ and $u_{N+1} := u_1$.
- Let p_j be the unique polynomial of degree ≤ 2 with $p_j(x_{j-1}) = u_{j-1}$, and $p_j(x_{j+1}) = u_{j+1}$, and $p_j(x_j) = u_j$.
- Set $w_j = p'_j(x_j)$. This is the second-order, centered, approximation to $u'(x_j)$.
- Discrete differentiation (a finite dimensional linear operator) representable by a matrix.
- Tridiagonal, Toeplitz, circulant matrix.



Comparison of Finite Difference, Finite Element, and Spectral Methods

Spectral One high-order polynomial for WHOLE domain



Finite Difference Multiple Overlapping Low-Order Polynomials



Finite Element/Spectral Element Non-Overlapping Polynomials, One per Subdomain





From Finite Differences to Spectral Methods

- Higher order finite difference schemes have matrices of higher bandwidth.
- Spectral methods: "infinite order" finite difference methods with matrices of infinite bandwidth (on unbounded/periodic domains).



Continuous Fourier Transforms

• Fourier transform:

$$\hat{u}(k) = \int_{-\infty}^{\infty} u(x) e^{-ikx} dx, \quad k \in \mathbb{R}$$

• Inverse Fourier transform:

$$u(x) = rac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}(k) e^{ikx} dk, \quad x \in \mathbb{R}$$

 \bullet continuous, unbounded \leftrightarrow unbounded, continuous



Semidiscrete Fourier Transforms

- Wavenumber domain a bounded interval of length $2\pi/h$, where h is uniform grid spacing
- Semidiscrete Fourier transform:

$$\hat{v}(k) = h \sum_{j=-\infty}^{\infty} v_j e^{-ikx_j}, \quad k \in [-\pi/h, \pi/h]$$

• Inverse Semidiscrete Fourier transform:

$$m{v}_j = rac{1}{2\pi} \int_{-\pi/h}^{\pi/h} \hat{v}(k) e^{ikx_j} dk, \quad j \in \mathbb{Z}$$

 \bullet discrete, unbounded \leftrightarrow bounded, continuous



Aliasing

- Consider f and g over \mathbb{R} defined by $f(x) = e^{ik_1x}$ and $g(x) = e^{ik_2x}$.
- f and g are equal over \mathbb{R} iff $k_1 = k_2$.
- Consider restrictions of f and g to $h\mathbb{Z}$ defined by $f_j = e^{ik_1 x_j}$ and $g_j = e^{ik_2 x_j}$.
- f and g are equal over $h\mathbb{Z}$ iff $k_1 k_2$ is an integer multiple of $2\pi/h$.
- For any Fourier mode e^{ikx} there are infinitely many others (known as its "aliases") that match it on a uniform grid.



Discrete Fourier Transforms

- Assume *N*, number of grid points, even.
- Assume function u periodic with period 2π on $[0, 2\pi]$.
- Assume uniform grid spacing $h = 2\pi/N$.
- Discrete Fourier transform (DFT):

$$\hat{v}_k = h \sum_{j=1}^N v_j e^{-ikx_j}, \quad k \in \{-N/2 + 1, \dots, N/2\}$$

• Inverse Discrete Fourier transform:

$$v_j = rac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} \hat{v}_k e^{ikx_j}, \quad j \in \{1, \dots, N\}$$

 \bullet discrete, bounded \leftrightarrow bounded, discrete



Fourier Transforms, cont'd





Band-Limited Interpolant for Discrete Case

• "Think globally. Act locally."

Define a trigonometric interpolant by evaluating the formula for inverse discrete Fourier transform for x ∈ ℝ rather than just x_j ∈ {h, 2h, ..., 2π − h, 2π} and correct the asymmetry in highest wavenumber by noting that v̂(−N/2) = v̂(N/2) (due to periodicity) to get:

$$p(x) = rac{1}{2\pi} \sum_{k=-N/2}^{\prime N/2} \hat{v}_k e^{ikx}, \quad x \in [0, 2\pi]$$

• Prime means divide first and last terms by two. That will produce a cos(Nx/2).



Band-Limited Interpolant for Discrete Case, cont'd

- Periodic grid function as a linear combination of periodic Kronecker delta functions: $v_j = \sum_{m=1}^{N} v_m \delta_{j-m}$.
- Band-limited trigonometric interpolant of periodic Kronecker delta (previous sum for $\hat{v}_k = h$)

$$p_{\delta}(x) = rac{\sin(\pi x/h)}{(2\pi/h) \tan(x/2)} =: \operatorname{psinc}_N(x)$$

- Band-limited interpolant in terms of psinc: $p(x) = \sum_{m=1}^{N} v_m \operatorname{psinc}_N(x - x_m)$
- Set $w_j = p'(x_j)$. This is an spectral approximation to $u'(x_j)$.
- Differentiation operator matrix in Cartesian basis D_N = toeplitz ½[···, cot(2h/2), -cot(1h/2), 0, cot(1h/2), -cot(2h/2), ····]



FFT

FFT Implementation of Fourier Spectral Methods

- Compute \hat{v} from v.
- Define $\hat{w}_i = (ik)^r \hat{v}_k$ (Fourier diagonalizes differentiation) but $\hat{w}_{N/2} = 0$ if r is odd.
- Compute w from \hat{v} .
- Note: FFTW, used in MATLAB and many other packages, stores wavenumbers in a different order than used here; that order in this notation becomes: 0:N/2-1 0 -N/2+1:-1



FFT Fun Facts

- FFT should probably be called "FGT." What we now know as FFT was discovered by Gauss when he was 28 (in 1805). Fourier completed his first big article two years after that! Gauss wrote on the subject but he did not publish it.
- Cooley and Tukey rediscovered FFT in 1965.



Regularity of Function and Accuracy of Fourier Spectral Methods

- Regularity transforms to decay, because more regularity means slower changes in the function, which in turn mean less energy at higher wavenumbers.
- A rapidly decaying Fourier transform means small errors due to discretizations, because these errors are caused by aliasing of higher wavenumbers to lower ones.



Regularity Transforms to Decay

- (a) If u has r-1 continuous derivatives in $L^2(\mathbb{R})$ for some $r \ge 0$ and an rth derivative of bounded variation, then $\hat{u}(k) = O(|k|^{-r-1})$ as $|k| \to \infty$.
- (b) If *u* has infinitely many continuous derivatives in $L^2(\mathbb{R})$, then $\hat{u}(k) = O(|k|^{-m})$ as $|k| \to \infty$.
- (c) If there exist a, c > 0 such that u can be extended to an analytic function in the complex strip |Im z| < a with ||u(. + iy)|| ≤ c uniformly for all y ∈ (-a, a), then u_a ∈ L²(ℝ), where u_a(k) = e^{a|k|} û(k). The converse also holds.
- (d) If u can be extended to an entire function and there exist a > 0 such that |u(z)| = o(e^{a|z|}) as |z| → ∞ for all z ∈ C, then û has compact support contained in [-a, a].



Regularity Transforms to Decay, Examples

(a) with
$$r = 0$$
 $s(x) = \frac{1}{2}\chi_{[-1,1]}$ $\hat{s}(k) = sin(k)/k$
(a) with $r = 1$ $s * s(x)$ $\hat{s * s}(k) = (sin(k)/k)^2$
(c) and (a) with $r = 1$ $u(x) = \frac{\sigma}{x^2 + \sigma^2}$ $\hat{u}(k) = \pi e^{-\sigma |k|}$
"between" (c) and (d) $e^{-x^2/2\sigma^2}$ $\hat{u}(k) = \sigma\sqrt{\pi/2}e^{-\sigma^2k^2/2}$



Spectral Approximation to Derivatives of Hat Function and $e^{sin(x)}$





Finite Difference Approximation to Derivative of $e^{sin(x)}$





Fourier Spectral Approximation to Derivative of $e^{sin(x)}$





Theorem

Poisson summation (aka Aliasing) Let $u \in L^2(\mathbb{R})$ have a first derivative of bounded variation, and let v be the grid function on $h\mathbb{Z}$ defined by $v_j = u(x_j)$. Then for all $k \in [-\pi/h, \pi/h]$,

$$\hat{v}(k) = \sum_{j=-\infty}^{\infty} \hat{u}(k+2\pi j/h)$$

• Bring $\hat{u}(k)$ to LHS. All other modes amount to aliasing error.



Accuracy of Fourier Spectral Derivative

Let $u \in L^2(\mathbb{R})$ have a ν th derivative ($\nu \ge 1$) of bounded variation and let w be the ν th spectral derivative of u on the grid $h\mathbb{Z}$. The following hold uniformly on the grid.

- (a) If u has r-1 continuous derivatives in $L^2(\mathbb{R})$ for some $r \ge \nu + 1$ and an rth derivative of bounded variation, then $|w_j - u^{(\nu)}(x_j)| = O(|h|^{r-\nu})$ as $h \to 0$.
- (b) If u has infinitely many continuous derivatives in $L^2(\mathbb{R})$, then $|w_j u^{(\nu)}(x_j)| = O(|h|^m)$ as $h \to 0$, for every $m \ge 0$.
- (c) If there exist a, c > 0 such that u can be extended to an analytic function in the complex strip |Im z| < a with ||u(. + iy)|| ≤ c uniformly for all y ∈ (-a, a), then |w_j u^(ν)(x_j)| = O(e^{-π(a-ε)/h}) as h → 0 for every ε > 0.
- (d) If u can be extended to an entire function and there exist a > 0 such that |u(z)| = o(e^{a|z|}) as |z| → ∞ for all z ∈ C, then, provide h ≤ π/a, w_j = u^(ν)(x_j).





Variable Coefficient Wave Equation

- Consider $u_t + c(x)u_x = 0$, $c(x) = 1/5 + \sin^2(x-1)$ for $x \in [0, 2\pi]$, t > 0, with periodic boundary conditions and initial condition $u(x,0) = e^{-100(x-1)^2}.$
- For time derivative use a leap frog scheme and approximate spatial derivatives spectrally.
- Leap frog needs two initial conditions to start. PDE gives one. For simplicity, extrapolate backwards assuming constant wavespeed of 1/5. (Could use a one-step formula like Runge–Kutta to start off leap frog.)



Wave PDE, Spectral Spatial Discretization and Leap Frog Time Marching Code

```
N = 128; h = 2*pi/N; x = h*(1:N); t = 0; dt = h/4;
c = .2 + sin(x-1).^{2};
v = \exp(-100*(x-1).^{2}); vold = \exp(-100*(x-.2*dt-1).^{2});
```

```
tmax = 8; tplot = .15; clf, drawnow
plotgap = round(tplot/dt); dt = tplot/plotgap;
nplots = round(tmax/tplot);
data = [v; zeros(nplots,N)]; tdata = t;
```



Wave PDE Code, Cont'd

```
for i = 1:nplots
    for n = 1:plotgap
        t = t + dt;
        v_hat = fft(v);
        w_{hat} = 1i * [0:N/2-1 \ 0 \ -N/2+1:-1] \ .* \ v_{hat};
        w = real(ifft(w_hat));
        vnew = vold - 2*dt*c.*w; vold = v; v = vnew;
    end
    data(i+1,:) = v; tdata = [tdata; t];
end
```



Wave Propagation



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Direct vs. Inverse Modeling

- Direct: Based on First Principles (Fundamental/Constitutive laws).
- Inverse: Data Driven (Process Control, Fault Diagnosis, Reverse Engineering of Gene Regulatory Networks).



Drawbacks of Direct Modeling

- Not all first principles known for complex systems.
- Full set of Initial/Boundary Conditions not available.
- Discrepancy between prediction of model and behavior of system due to simplifying assumptions (Inadequate Parameters) in modeling.



PDE Reconstruction based on Regression

- Regression: Parameter equations derived from discretized PDE directly.
- Benefits: Relatively low computational cost; generalizability to multiple dimensions.
- Downsides: Relatively high resolution data demands; noise prune.



Identification of Partial Differential Equations

- Mathematical structure: a nonlinear monomial basis PDE containing all linear combinations of the monomials up to a certain derivative order and nonlinearity degree (Volterra Model).
- Temporal and spatial discretization, the latter using spectral methods, leads to an over-determined system of linear algebraic equations $A\alpha = b$ whose unknowns α are the parameters we seek.



Structure Selection using Least Squares with QR Decomposition

- With zero mean white noise, this gives maximum-likelihood estimate (MLE) of parameters.
- Orthonormal basis vectors in Q allow error reduction resulting from each parameter to be calculated independently.
- With no parameters maximum (squared) error would be $b^T b$.
- Addition of every parameter α_j leads to an error reduction of β_j^2 where $R\alpha = \beta$ and $Q\beta = b$.
- Error Reduction Ratio (ERR) $\beta_j^2/b^T b$.



Reconstruction of Kuramoto–Sivashinsky PDE

•
$$u_t = -uu_x - u_{xx} - \epsilon u_{xxx}, \quad (x, t) \in I \times \mathbb{R}^+$$

• $u(x,0) = u_0(x), u(x+L,t) = u(x,t)$

•
$$I = [0, L), L = 32\pi, \epsilon = 1, u_0(x) = cos(x/16)(1 + sin(x/16))$$

- Simulated till t = 150s with exponential time differencing for time marching and spectral methods for spatial discretization.
- Assume a degree of nonlinearity 2 and a highest order of spatial derivative of 4, giving a total number of 28 monomials in the model structure. Structure selection (SS), aka model reduction, means omit parameters with ERR less than a threshold. Here ERR threshold 0.5%.



KS Evolution





PDE Reconstruction

KS Parameters Identified

Case:	Δt =0.1; No SS		$\Delta t=0.1$; with SS		$\Delta t=0.01$; No SS		$\Delta t = 0.01$; with SS	
Terms	Finite diff.	Spectral	Finite diff.	Spectral	Finite diff.	Spectral	Finite diff.	Spectral
1	0.000 148 98	0.000 001 89	0	0	0.000 135 00	0.000 000 36	0	0
х	-0.000 010 28	0.000 000 02	0	0	$-0.000\ 009\ 88$	-0.000 000 02	0	0
и	-0.000 164 57	-0.000 007 53	0.001 737 9	1.922×10^{-07}	-0.000 135 66	-0.000 000 64	0.001 964 623	2.49966×10^{-08}
u _x	-0.000 178 99	0.000 002 03	0	0	-0.000 204 27	0.000 000 28	0	0
u _{xx}	-1.007 107 97	-1.000 032 95	-0.951 403	-1	-1.006 990 37	-1.000 003 09	-0.952 312 176	$-1.000\ 000\ 014$
u _{xxx}	0.000 246 72	0.000 004 38	0	0	0.000 230 69	0.000 000 25	0	0
u _{xxxx}	-1.007 933 44	$-1.000\ 015\ 26$	-0.974 14	$-1.000\ 001$	-1.007 983 05	-1.000 001 29	-0.974 721 479	$-1.000\ 000\ 014$
x^2	0.000 000 10	0.000 000 00	0	0	0.000 000 10	0.000 000 00	0	0
хи	-0.000 006 10	0.000 000 22	0.000 101 1	4.169×10^{-09}	-0.000 006 57	0.000 000 01	$9.587~02 \times 10^{-05}$	-4.75549×10^{-10}
xu_x	0.000 003 04	0.000 000 06	0	0	0.000 003 06	0.000 000 00	0	0
xu _{xx}	-0.000 002 98	0.000 000 81	0	0	-0.000 006 52	0.000 000 02	0	0
xuxxx	0.000 001 55	0.000 000 04	0	0	0.000 001 50	0.000 000 00	0	0
XU _{3Nex}	0.000 022 45	0.000 000 47	0	0	0.000 021 53	0.000 000 00	0	0
u2"13"	-0.000 046 83	-0.000 001 76	0	0	-0.000 034 92	-0.000 000 11	0	0
uux	-1.004 459 88	-0.999 984 02	-1.048 316	-1.000003	-1.004 423 62	-0.999 998 03	-1.048 476 897	-1.000 000 016
uurr	-0.000 549 26	-0.000 012 35	0	0	-0.000 458 45	-0.000 000 78	0	0
uuxxx	-0.003 698 95	0.000 028 57	-0.063 258	0	-0.003 587 34	0.000 002 22	-0.062 982 54	0
uurm	-0.000 638 07	-0.000 004 77	0	0	-0.000 629 70	-0.000 000 17	0	0
u_r^2	-0.000 328 89	-0.000 008 20	0	0	-0.000 335 34	0.000 000 25	0	0
<i>u_xu_{xx}</i>	-0.011 878 19	-0.000 011 02	-0.141 359	0	-0.011 545 27	0.000 010 40	-0.141 473 438	0
u _x u _{xxx}	-0.000 321 00	-0.000 019 25	0	0	-0.000 308 79	0.000 000 09	0	0
$u_x u_{xxxx}$	0.044 568 47	-0.000 003 94	0	0	0.044 720 38	0.000 005 47	0	0
u_{rr}^2	-0.000 078 35	-0.000 002 53	0	0	0.000 031 72	-0.000 000 76	0	0
<i>u</i> ₁₁ <i>u</i> ₁₁₁	0.096 215 67	0.000 040 08	0	0	0.096 464 44	0.000 006 37	0	0
$u_{rr}u_{rrrr}$	-0.000 753 60	-0.000 006 95	0	0	-0.000 707 04	-0.000 000 38	0	0
u_{rrr}^2	-0.000 172 71	-0.000 010 76	0	0	-0.000 159 49	-0.000 000 08	0	0
u,,u,	0.024 956 64	0.000 012 95	0	0	0.025 065 17	0.000 003 89	0	0
u_{xxxx}^2	-0.000 197 52	-0.000 002 95	0	0	-0.000 187 86	$-0.000\ 000\ 08$	0	0



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Algebraic Polynomial Interpolation

- Fourier was for periodic domains. What to do for nonperiodic domains?
- Periodic extension? Not unless solutions is exponentially close to a constant, because smooth becomes nonsmooth leading to global contamination (Gibbs phenomenon)—error in interpolant O(1), error in derivative O(N), etc.
- Solution: Replace trigonometric polynomials with algebraic ones. What about the grid? Equispaced leads to Runge's phenomenon. Use clustered grids with density asymptotic to $\mu(x) = N/\pi\sqrt{1-x^2}$.
- Distance between adjacent nodes approximately $1/\mu(x)$. Average spacing $O(N^{-2})$ near end points and $O(N^{-1})$ in the interior.



Chebyshev Polynomials

• Explicit equation $T_n(x) = cos(ncos^{-1}(x))$

• Extrema at
$$x = cos(k\pi/n), k = 0:n$$

• Zeros at
$$x = cos((k + 1/2)\pi/n), k = 0 : n - 1$$

• Difference equation $T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$, $T_0(x) = 1, T_1(x) = x$



Chebyshev Polynomial Graphs in $\left[-1,1\right]$





Algebraic Polynomial Interpolation in Equispaced and Chebyshev Points for $u(x) = 1/(1 + 16x^2)$





Node Density and Potential Function

• $|p(z)| = e^{N\phi_N(z)}$, where $\phi_N(z) = N^{-1}\sum_{j=1}^N \log|z-z_j|$

•
$$\phi(z) = \int_{-1}^{1} \rho(x) \log |z - x| dx$$

- Equispaced nodes, uniform distribution $\rho(x) = 1/2, x \in [-1, 1]$. $\phi(0) = -1$ and $\phi(\pm 1) = -1 + \log(2)$
- Chebyshev nodes, Chebyshev distribution $\rho(x) = 1/\pi\sqrt{1-x^2}, x \in [-1,1]$. $\phi(x) = -\log(2)$ for all $x \in [-1,1]$



Polynomials and their Equipotential Curves





Chebyshev Spectral Derivative Matrix





Chebyshev Spectral Derivative Matrix, Values

$D_5 =$

8.5000	-10.4721	2.8944	-1.5279	1.1056	-0.5000
2.6180	-1.1708	-2.0000	0.8944	-0.6180	0.2764
-0.7236	2.0000	-0.1708	-1.6180	0.8944	-0.3820
0.3820	-0.8944	1.6180	0.1708	-2.0000	0.7236
-0.2764	0.6180	-0.8944	2.0000	1.1708	-2.6180
0.5000	-1.1056	1.5279	-2.8944	10.4721	-8.5000



Chebyshev Spectral Derivative Matrix, Bar Plot





Chebyshev Spectral Derivative of $e^x sin(5x)$





Accuracy of Chebyshev Spectral Derivative

- Define $\phi_{[-1,1]} = \sup\{\phi(x) : x \in [-1,1]\}$
- If there exists a constant $\phi_u > \phi_{[-1,1]}$ such that u is analytic throughout the closed region $\{z \in \mathbb{C} : \phi(z) \le \phi_u\}$, then there exists a constant C > 0 such that for all $x \in [-1,1]$ and all N, $|u^{(\nu)}(x) p_n^{(\nu)}(x)| \le e^{-N(\phi_u \phi_{[-1,1]})}$, for any $\nu \ge 0$



Accuracy of Chebyshev Spectral Derivative





Allen-Cahn PDE

Allen–Cahn Reaction–Diffusion PDE

- $u_t = au_{xx} + u u^3, u(-1, t) = -1, u(1, t) = 1$
- Direct: $a = 0.01, N = 100, t = 70, \Delta t = 1/8$
- Inverse: Use states up to t = 35; assume degree of nonlinearity 3 and order 2, leading to 20 terms to be identified.



Allen-Cahn PDE, Solution





Allen-Cahn PDE, Identification

	Coefficients						
	With	n SR	Without SR				
Terms	FD	CGL	FD	CGL			
1	0	0	0.027 738 81	0.000 000 00			
и	0.845 904 95	1.000 001 81	0.923 294 32	0.999 815 99			
u_x	0	0	$-0.002\ 673\ 48$	0.000 000 00			
u_{xx}	0.008 173 80	0.010 000 01	0.009 152 51	0.009 998 03			
u^2	0	0	-0.027 701 45	0.000 000 00			
uu_x	0.017 813 28	$-0.000\ 000\ 02$	0.000 527 72	$-0.000\ 015\ 75$			
uu _{xx}	0	0	0.001 467 72	0.000 000 00			
u_x^2	0	0	-0.001 062 96	0.000 000 00			
$u_x u_{xx}$	0.000 168 97	0.000 000 00	0.000 023 09	$-0.000\ 000\ 14$			
u_{xx}^2	0	0	0.000 003 59	0.000 000 00			
u^3	$-0.846\ 204\ 82$	$-1.000\ 001\ 88$	-0.923 199 28	-0.999 815 88			
$u^2 u_x$	0.003 447 08	0	0.013 085 69	0.000 000 00			
$u^2 u_{xx}$	0.001 934 32	0	0.000 887 16	$-0.000\ 001\ 10$			
uu_x^2	0.003 088 25	0	0.004 015 88	0.000 008 59			
$uu_x u_{xx}$	0	0	-0.000 364 33	0.000 000 00			
uu_{xx}^2	0	0	0.000 008 13	$-0.000\ 000\ 03$			
u_x^3	0	0	0.000 004 85	0.000 000 00			
$u_x^2 u_{xx}$	0	0	0.000 000 22	0.000 000 10			
$u_x u_{xx}^2$	0	0	$-0.000\ 000\ 80$	0.000 000 00			
u_{xx}^3	0	0	$-0.000\ 000\ 03$	0.000 000 00			



Allen–Cahn PDE, Error in Dominant Coefficients vs. Error Reduction Ratio





Allen-Cahn PDE, Prediction and Prediction Error





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