Motivation

- model: Q-tensor model of nematic liquid crystal cell
- aim: model dynamics of defect movement
- problem: characteristic lengths with large scale differences
- uniform grid: many grid points needed to capture defect behaviour
- idea: use adaptive grid methods to ensure there is no waste of computational effort

Moving Mesh Method

existing node points moved to regions of high error

map from physical domain $x \in [0, 1]$ to computational domain $\xi \in [0, 1]$ based on equidistribution principle

$$M(u(x,t)) = \sqrt{\gamma + \left(\frac{\partial u(x,t)}{\partial x}\right)^2}$$

monitor function
arc-length of solution u

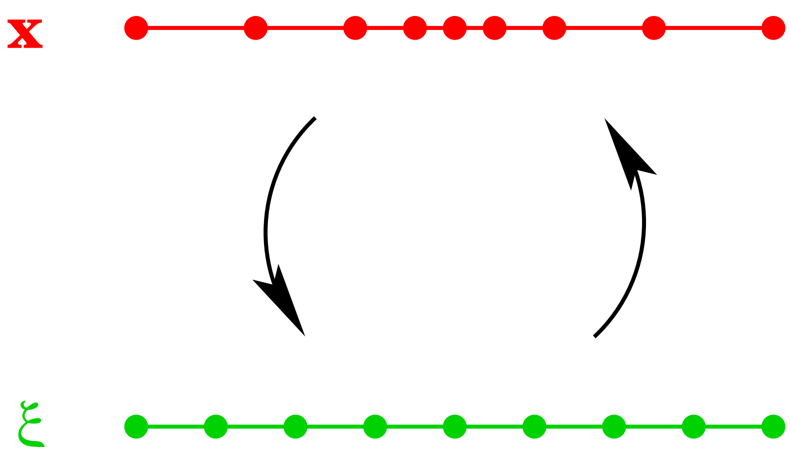
equidistribution principle

$$\int_0^{x(\xi,t)} M(s,t)\,ds = \xi \int_0^1 M(s,t)\,ds$$

Sanz-Serna and Christie, JCP 67, 1986

adapted mesh on physical domain

$$0 = x_0 < x_1 < \ldots < x_{N-1} < x_N = 1$$



mapping

$$x = x(\xi, t) \quad , \quad \xi \in [0,1],$$
$$x(0,t) = 0 \quad , \quad x(1,t) = 1$$

$$\xi_i = \frac{i}{N}, \qquad i = 0, 1, \ldots, N, \qquad N \in \mathbb{Z}^+$$

uniform mesh on computational domain

1D Nematic Model Problem

symmetric traceless Q-tensor

$$Q = \begin{bmatrix} q_1 & q_2 & q_3 \\ q_2 & q_4 & q_5 \\ q_3 & q_5 & -q_1 - q_4 \end{bmatrix}$$

homogeneous and uniaxial region of length d

$$Q = \sqrt{\frac{3}{2}} S \begin{bmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{2}{3} \end{bmatrix}$$

Q depends only on scalar order parameter S

minimise free energy desity

$$\mathcal{F} = \int_V F(q_i, \nabla q_i)\, dV$$

Euler-Lagrange equation

$$S'' = \alpha S - \beta S^2 + \gamma S^3$$

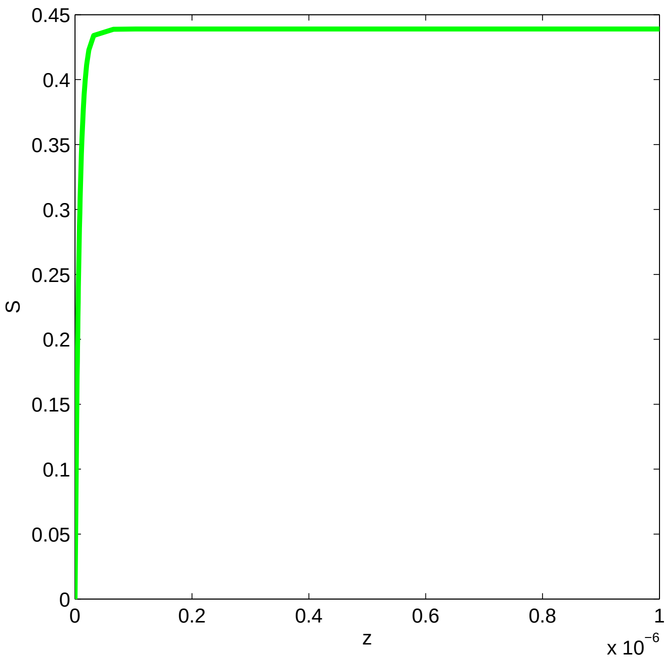
α, β, $\gamma > 0$

boundary conditions

$$S = 0 \quad \text{at} \quad z = 0,$$

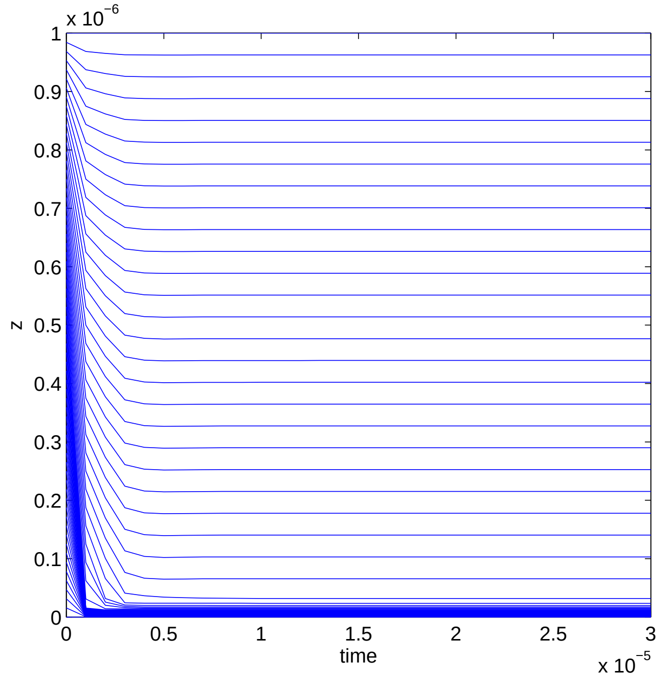
$$S = S_{eq} \quad \text{at} \quad z = d$$

$S_{eq} \equiv S$ at equilibrium



solution with $d = 1\ \mu$m

boundary layer at $z = 0$



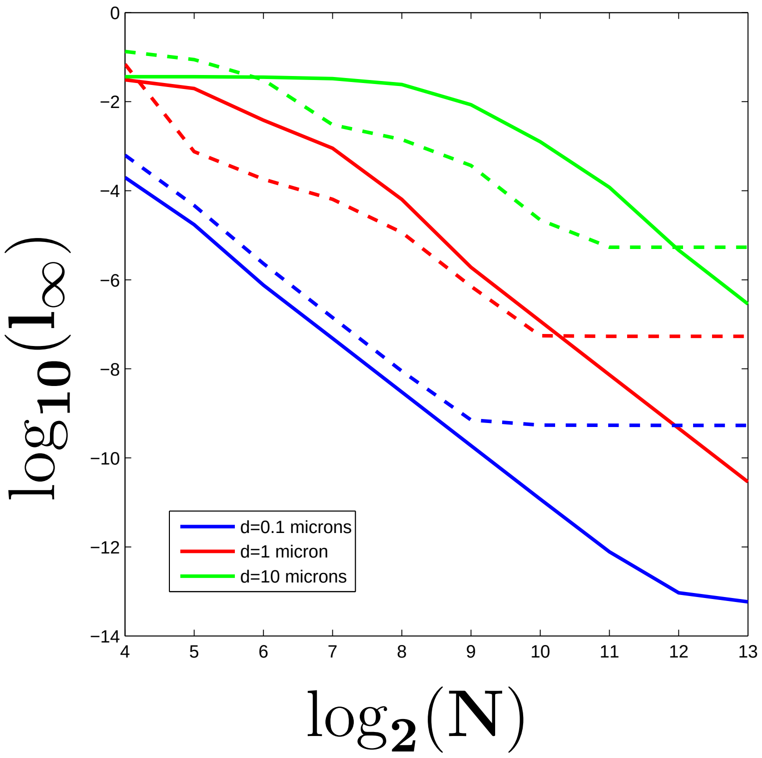
node paths based on equidistribution

monitor function $M(S(z,t)) = \sqrt{1 + \left(\frac{dS}{dz}\right)^2}$

accuracy: measuring errors

measure of error $\boxed{l_\infty = \max_{j=0,\ldots,N/2} |S_f(z_j) - S_N(z_j)|}$

S_f on very fine uniform grid, S_N on grid with N points

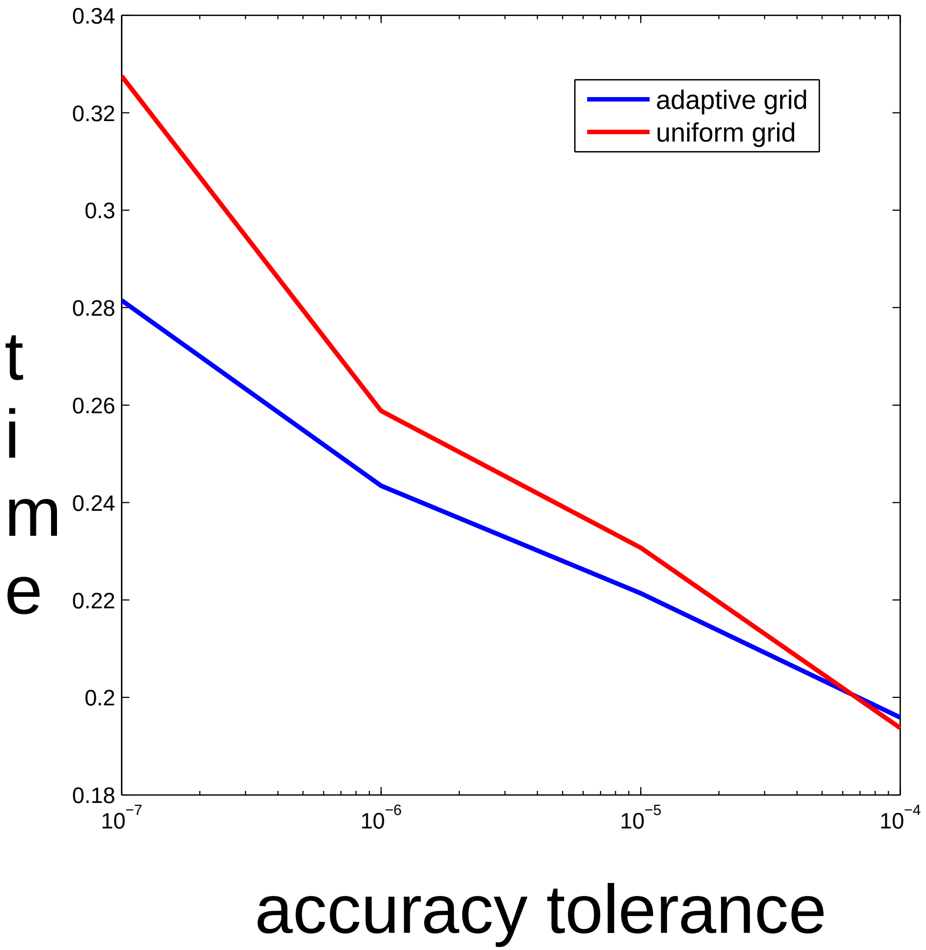


uniform grid: solid line
adaptive grid: dashed line

adaptive grid has smaller error for fixed number of grid points when effect of boundary layer is more pronounced

error measure contaminated by interpolation issues for adaptive grid due to very small elements

efficiency: CPU times (in seconds)



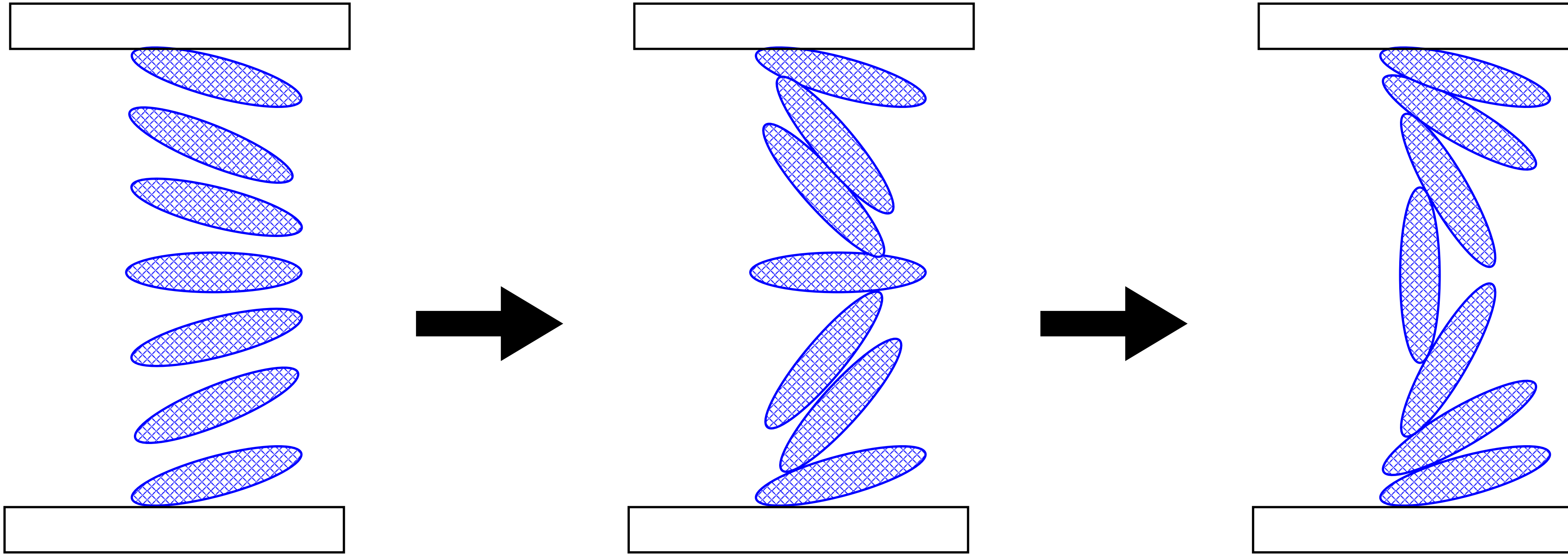
% gain in time

$$\frac{\text{adaptive} - \text{uniform}}{\text{uniform}}$$

tol	N_{uni}	N_{ad}	% gain
1×10^{-4}	174	115	-1.13
1×10^{-5}	338	258	4.05
1×10^{-6}	568	476	5.94
1×10^{-7}	1051	817	14.05

Order Reconstruction: Pi-cell

Barberi et al. Eur. J. Phys. E (2004)



horizontal

H-state

intermediate

I-state

vertical

V-state

H-V transition (via I) induced by vertical electric field

order reconstruction at cell centre

no longer purely uniaxial: need full Q-tensor

5 coupled PDEs for q_is
$+$
PDE for electric potential U

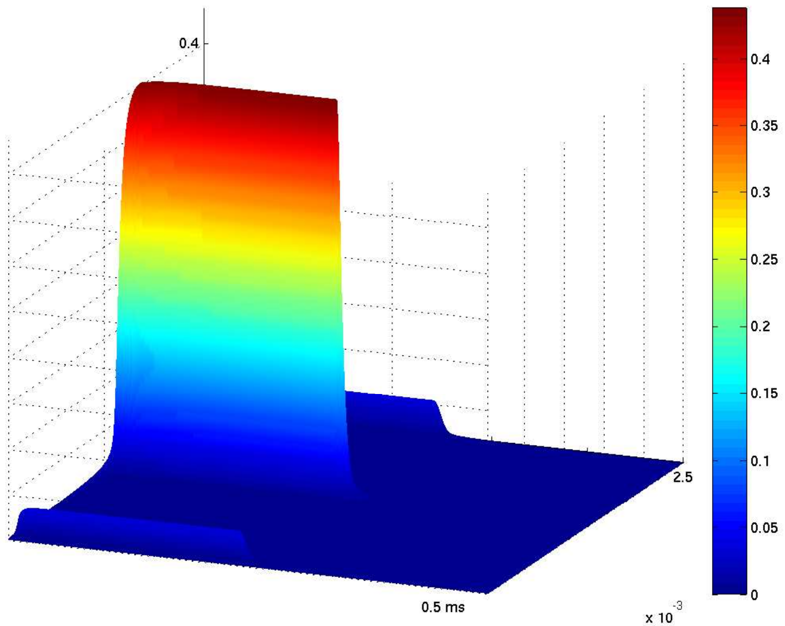
$$M(T(z,t)) = \sqrt{1 + \left(\frac{dT}{dz}\right)^2}$$

monitor function
based on $T(z,t) = \mathrm{tr}(Q^2)$

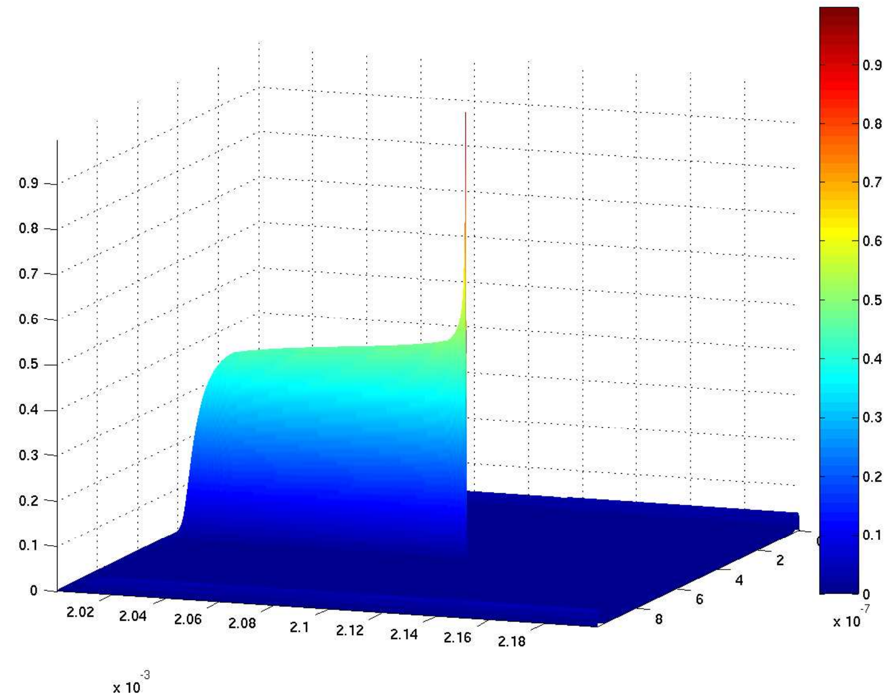
measure of
biaxiality

$$b = \sqrt{1 - \frac{6\,\mathrm{tr}(Q^3)^2}{\mathrm{tr}(Q^2)^3}}$$

solutions for electric field strength V just below and above the critical voltage at which switching occurs



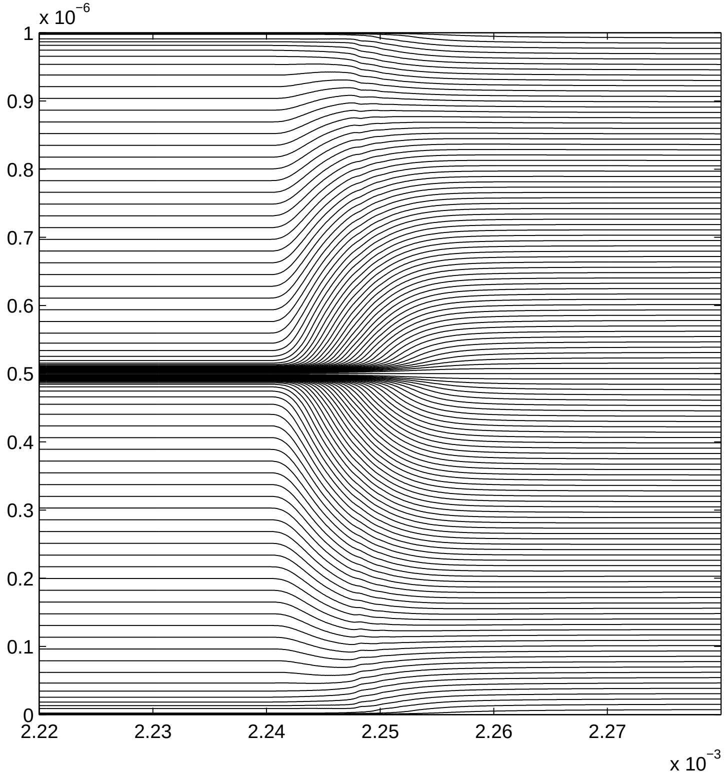
$V = 11.3$



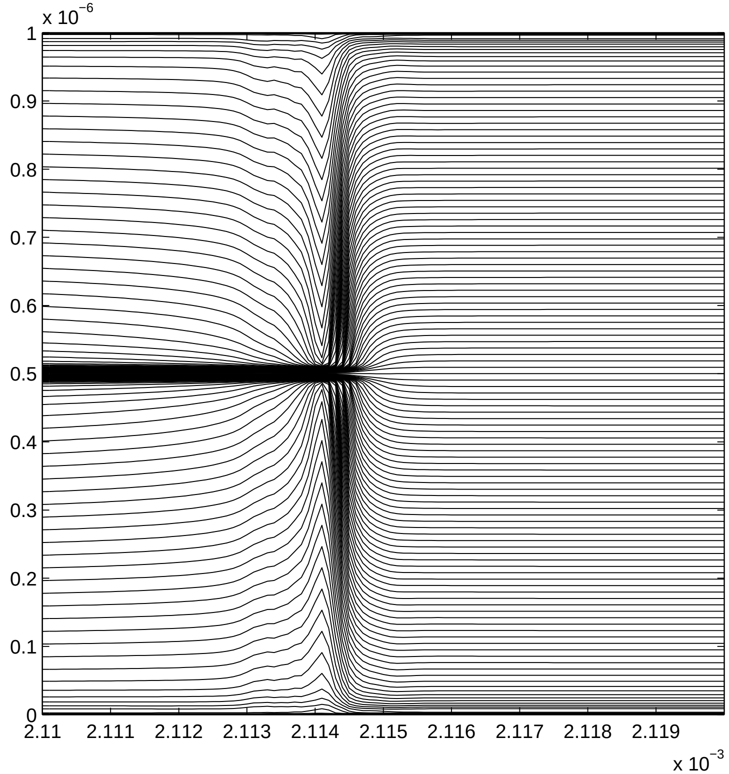
$V = 11.32$

adaptive grid with 256 quadratic elements

grid trajectories



$V = 11.3$



$V = 11.32$

$\sim 25\%$ fewer points/less CPU time with adaptive grid

wrong switching voltage identified if uniform grid is not fine enoug

Conclusions

- monitor function: arc-length monitor function based on $tr(Q^2)$ appears to work well
- accuracy: to obtain a specified level of accuracy, adaptive grid requires fewer points
- efficiency: cost of calculating moving mesh is not prohibitive
- WARNING: inaccurate results can be obtained if uniform grid used is not fine enough
- the future: study of Moving Mesh PDEs in two dimensions underway…

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