

MD:

$X_i(t)$

$$E = \frac{1}{2} \sum_{i \neq j} \varphi(|X_i(t) - X_j(t)|)$$

$$m \ddot{x}_j(t) = f_j(t) = -\nabla_{x_j} E$$

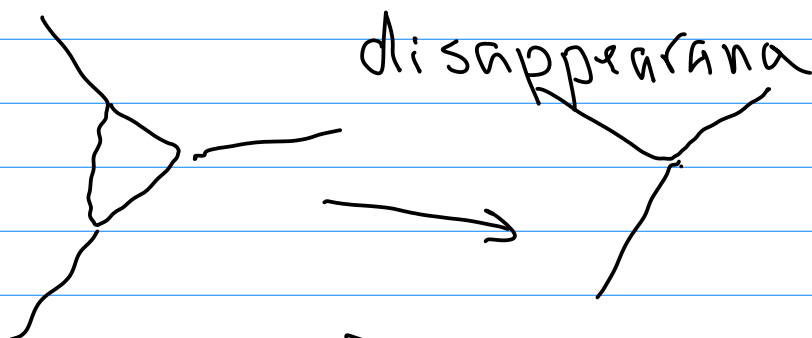
MC:

$$H = \sum_{\langle ij \rangle} J_{ij} (\delta_{s_i s_j} - 1) \quad s_i = \pm 1$$

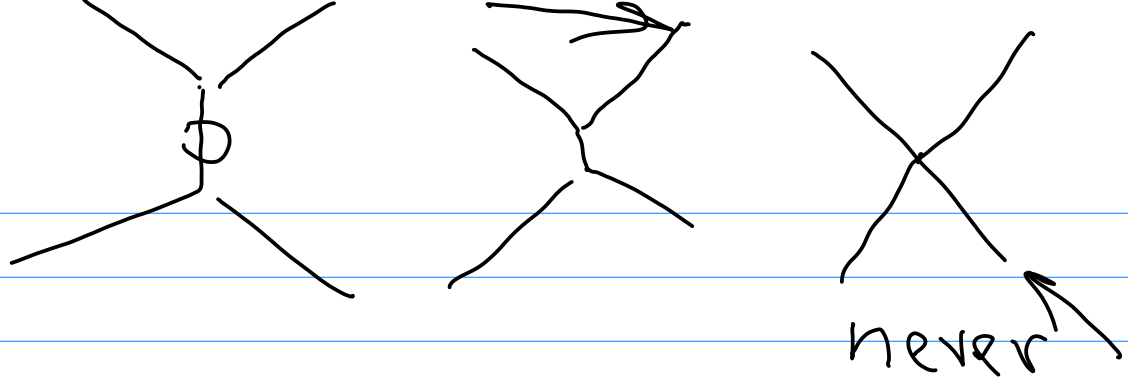
$$\bar{H} = \sum_{ij} J_{ij} (s_i - s_j)^2 = H + \text{const} \quad s_i^2 = 1$$

$$s_i - s_j \approx \nabla s$$

$$I = \int (s_i^2 - 1)^2 dx + \frac{1}{2} \int J |\nabla s|^2 dx$$



critical events

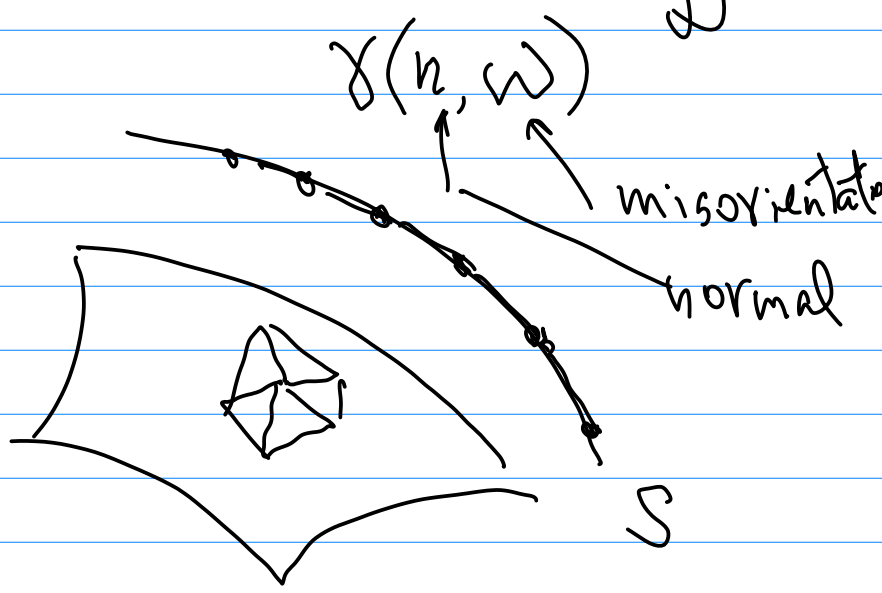


3D complicated.

Approx of PDE based models

γ energy GB

approx S
triangulation



$$E = \sum_j \int_{\Gamma_j} \gamma(n, w) ds \quad \text{total energy}$$

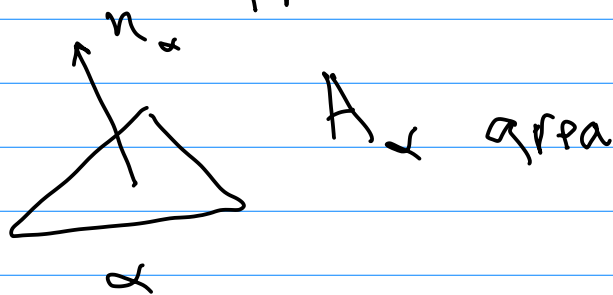
$$(1) \quad \sigma_n = -\mu \operatorname{div}_n (\nabla_n \gamma + \gamma n)$$

$n \in S^2$
 w rotation matrix
5 dim.

Discretization approx

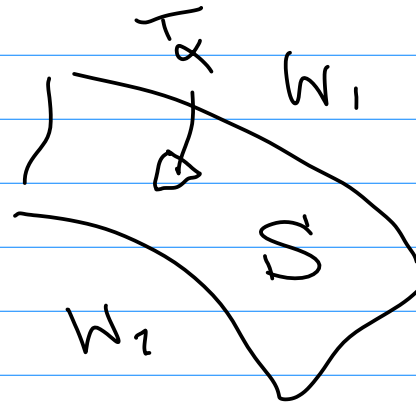
(2) To ensure energy dissipation

best to approx Ξ :



$$E(t) = \sum_{\alpha \in T} \chi(n_\alpha, \omega_\alpha) A_\alpha$$

T Triangulation.



$X_j(t)$ point on S .

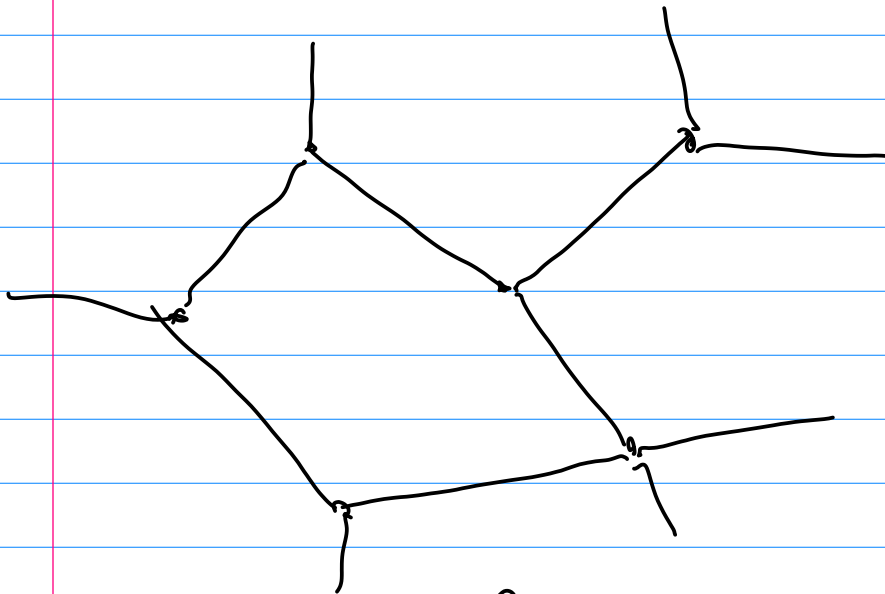
$$n_\alpha(t), A_\alpha(t): \sum_{\alpha} \chi(n_\alpha(t), \omega_\alpha) A_\alpha(t)$$

(2) $\frac{d}{dt} E(t) = \dots$ discretize (1).

gradient flow in L_2 $\int \frac{1}{\mu} v(x)^2 dx$

guarantees a good dissipation on discrete level !!

Vertex models 2D



all bd are straight.

Evolution?

$$E = \sum \delta(n, w) |x_i(t) - x_j(t)|$$

$$\frac{\delta E}{\delta t} = \dots \sum \langle \dot{x}_i, \cdot \rangle$$

norms: $\sum |\dot{x}_i|^2$

