

A message-passing scheme for non-equilibrium stationary states

NORDITA Seminar December 2, 2010

E.A., H. Mahmoudi (2010) [in preparation]

I. Neri, D. Bollé, J. Stat Mech. (2009) P08009 Y. Kanoria, A. Montanari (2009) arXiv:0907.0449

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Message-passing schemes are ways to approximately compute marginals of probability distributions.

In Artificial Intelligence known as Belief Propagation (BP); in Information Theory known as iterative decoding.



Bethe-Peierls approximation = Belief Propagation

JS Yedidia, WT Freeman, Y Weiss (2001) M Mézard, A Montanari Physics, Oxford University Press (2009)

Configuration space; N discrete variables

Cost or energy function; sum of local terms

Marginal (one-spin) probabilities

 $ec{s} \in \{1, ..., q\}^N$ $\mathcal{H}(ec{s}) = \sum_{a=1}^M e_a(ec{s}_a)$ $p_i(s_i) = rac{1}{Z} \sum_{ec{s} \setminus s_i} e^{-eta \, \mathcal{H}(ec{s})}$

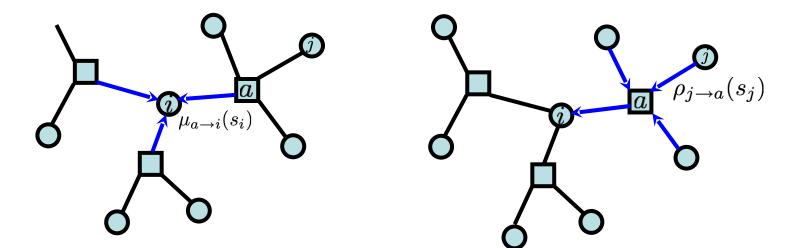
In statistical physics, artificial intelligence and information theory, such marginals (magnetizations, correlation functions etc) are typically what one wants to compute (or use)

$$\begin{cases} p(\vec{s}) \propto \frac{\prod_{a=1}^{M} p_a(\vec{s}_a)}{\prod_{i=1}^{N} (p_i(s_i))^{d_i-1}} & \blacksquare & Bethe-Peterls approximation \\ p_i(s_i) = \sum_{\vec{s}_a \setminus s_i} p_a(\vec{s}_a) & \blacksquare & Belief propagation \end{cases}$$



Factor graph representation illustrates canonical BP

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The 'messages" $\mu_{a
ightarrow i}(s_i)$ and $ho_{j
ightarrow a}(s_j)$ are Lagrange multipliers.

They enforce the conditions that the marginal probabilities p_a over the spins partaking in one interaction a, summed over all those spins except i, is the marginal probability p_i , over that last spin.

$$p_i(s_i) = D_i \prod_{a \in \partial i} \mu_{a \to i}(s_i)$$

$$\mu_{a \to i}(s_i) = C_{a \to i} \sum_{\vec{s}_a \setminus i} \exp\left(-\beta e_a(\vec{s}_a)\right) \prod_{j \in \partial a \setminus i} \rho_{j \to a}(s_j) \quad \bullet$$

 $\rho_{i \to a}(s_i) = D_{i \to a} \prod_{b \in \partial i \setminus a} \mu_{b \to i}(s_i)$

- Iterative procedure to find fixed points of BP equations
- Exact on trees and an approximation on loopy graphs
- No guarantee to converge

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Non-equilibrium is the domain of kinetic theory.

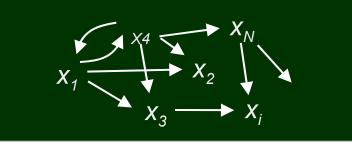
There is no Gibbs measure as there is in equilibrium.

But can one nevertheless compute marginals by a message-passing scheme?



Today's case study: diluted asymmetric spin glass

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S Kauffman (1969) J Hopfield (1982)

B Derrida (1987) A Crisanti, H Sompolinski (1988)and many others

$$\frac{d}{dt}p(\vec{\sigma}(t)) = W(t)\,p(\vec{\sigma}(t))$$

Fully asynchronous updates (master equations); not yet done

$$p(\vec{\sigma}(0)...\vec{\sigma}(t)) = \prod_{s=1}^{t} W[\vec{\sigma}(s) | \vec{h}(s)] p(\vec{\sigma}(0))$$
 Synchronous updates; which
can yet be varied in several
$$W[\vec{\sigma}(s) | \vec{h}(s)] = \prod_{i=1}^{N} \frac{\exp(\beta h_i(s) \sigma_i(s))}{2\cosh(\beta h_i(s))}$$
 ways (here in two ways)

$$h_i(t) = \sum_{j \in \partial i} c_{ji} J_{ji} \sigma_j(t-1) + \theta_i(t)$$

- parallel : simultaneously update all spins

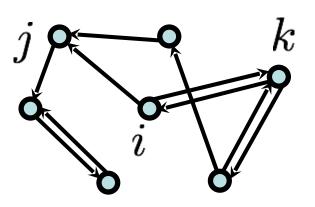
- sequential : one spin updated at a time

 $\sigma_i(t+1) = +1 \quad \text{with probability } \{1 + \exp(2\beta h_i(t))\}^{-1}$ $\sigma_i(t+1) = -1 \quad \text{with probability } \{1 + \exp(-2\beta h_i(t))\}^{-1}$ March 10, 2010 Erik Aurell, KTH Computational Biology



Dilution, asymmetry, and interaction strength

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 $\begin{array}{rcl} \text{connectivity} & \to & c \\ & \text{asymmetry} & \to & \epsilon \end{array}$

Derrida (1987) parametrization

connectivity
$$c_{ij} (i \rightarrow j)$$

$$p(c_{ij}) = \frac{c}{N} \delta_{c_{ij},1} + (1 - \frac{c}{N}) \delta_{c_{ij},0}$$

Starts as directed Erdős-Renyi graphs; where average connectivity would be *c*

Connections $i \to j$ and $j \to i$ dependent $p(c_{ji}|c_{ij}) = \epsilon \, \delta_{c_{ij},c_{ji}} + (1 - \epsilon) \, p(c_{ji})$

Gaussian or binary
$$J_{ij} \longrightarrow h_i(t) = \sum_{j \in \partial i} c_{ji} J_{ji} \sigma_j(t-1) + \theta_i(t)$$



Mean-field theory for magnetizations and correlations

$$p(\sigma_{i}(0), ..., \sigma_{i}(t)) = \sum_{\vec{\sigma} \setminus i(0), ..., \vec{\sigma} \setminus i(t)} p(\vec{\sigma}(0), ..., \vec{\sigma}(t)) \longrightarrow m_{i}(t)$$

$$p_{ij}(\sigma_{i}(0), ..., \sigma_{i}(t), \sigma_{j}(0), ..., \sigma_{j}(t')) = \sum_{\vec{\sigma} \setminus i, j(0), ..., \vec{\sigma} \setminus i, j(t)} p(\vec{\sigma}(0), ..., \vec{\sigma}(t))$$

$$\frac{d m_{i}(t)}{dt} = -m_{i}(t) + \langle \tanh(\beta H_{i}(t)) \rangle \xrightarrow{C_{ij}(t, t')} C_{ij}(t, t')$$

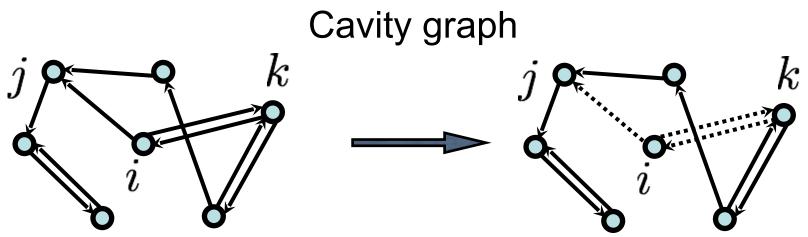
$$\frac{d c_{ij}(t, t')}{dt} = -c_{ij}(t, t') + \langle \tanh(\beta \sigma_{j}(t')H_{i}(t)) \rangle$$

$$\text{nMF} \quad m_{i} = \tanh \left[\beta(\sum_{j} J_{ji}m_{j} + \theta_{i})\right] \xrightarrow{C_{ij}(1 - m_{j})^{2}} \qquad \text{Crisanti, Sompolinski (1988)} \\ \text{Hertz et al (2010)} \\ \text{Hertz, Roudi arXiv:1001.6216}$$



Bethe - Peierls approximation for spin histories

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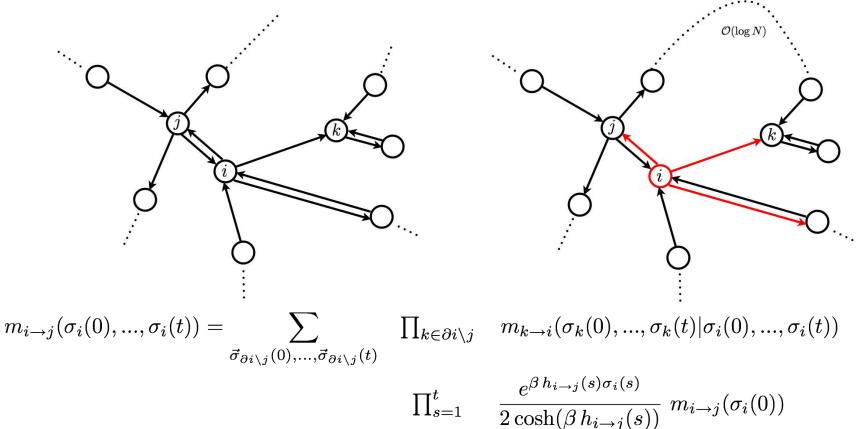
 $p(\vec{\sigma}(0)...\vec{\sigma}(t)) = p^{(i)}(\vec{\sigma}(0),...,\vec{\sigma}(t) | \sigma_i(0),...,\sigma_i(t)) \quad p_i(\sigma_i(0),...,\sigma_i(t))$

The cavity assumption: spins in cavity independent $p^i(\vec{\sigma}(0),...,\vec{\sigma}(t)|\sigma_i(0),...,\sigma_i(t)) = \prod_{k\in\partial i} m_{k\to i}(\sigma_k(0),...,\sigma_k(t)|\sigma_i(0),...,\sigma_i(t))$ The "messages" $m_{k\to j}$ are conditional probabilities



The (dynamic) cavity equation (parallel updates)

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In static (equilibrium) case this would be BP, Here history dependent, hence hard to use directly.



The time-factorized approximation (parallel updates)

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$$m_{i \to j}(\sigma_i(0), ..., \sigma_i(t)) = \prod_{s=0}^t m_{i \to j}(\sigma_i(s))$$

$$m_{i \to j}(\sigma_i(t)) = \sum_{\sigma_i(t-2), \vec{\sigma}_{\partial i \setminus j}(t-1)} \prod_{k \in \partial i \setminus j} m_{k \to i}(\sigma_k(t-1) | \sigma_i(t-2))$$

$$\frac{e^{\beta(\sum_{j \in \partial i} J_{ji} \sigma_j(t-1) + \theta_i)\sigma_i(t)}}{2\cosh(\beta(\sum_{j \in \partial i} J_{ji} \sigma_j(t-1) + \theta_i))} m_{i \to j}(\sigma_i(t-2))$$

(formally) time-dependent magnetization

I Neri, D Bolle (2009) Y Kanoria, A Montanari (2009)

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$$m_i(t) = \sum_{\vec{\sigma}_{\partial i}(t-1)} \prod_{j \in \partial i} m_{j \to i}(\sigma_j(t-1)) \tanh \left[\beta(\sum_{j \in \partial i} \frac{c_{ij}}{c} J_{ji} \sigma_j(t-1) + \theta_i) \right]$$



The sequential update model (poor man's Master eq.)

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$$\frac{dp(\vec{\sigma}(t))}{dt} = \sum_{i=1}^{N} \{ w_i (F_i \vec{\sigma}(t)) \ p(F_i \vec{\sigma}(t)) - w_i(\vec{\sigma})(t) \ p(\vec{\sigma})(t) \} \}$$

Fully asynchronous updates (Master equations) is not yet done. In sequential updates one (randomly picked) spin is updated at a time.

$$p(\vec{\sigma}(t)) = \sum_{\vec{\sigma}(t-1)} W(\vec{\sigma}(t) \,|\, \vec{\sigma}(t-1)) \, p(\vec{\sigma}(t-1))$$
$$W(\vec{\sigma}(t) \,|\, \vec{\sigma}(t-1)) = \delta_{\vec{\sigma}(t),\vec{\sigma}(t-1)} + \frac{1}{N} \sum_{i=1}^{N} \left\{ w_i(F_i \vec{\sigma}(t)) \,\delta_{\vec{\sigma}(t),F_i \vec{\sigma}(t-1)} - w_i(\vec{\sigma}(t)) \,\delta_{\vec{\sigma}(t),\vec{\sigma}(t-1)} \right\}$$

When N goes to infinity, it is reasonable to expect that sequential update tends to fully asynchronous updates. But at finite N there will be a difference.



The dynamic cavity equations for sequential updates

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The full dynamic cavity equations :

$$m_{i \to j}(\sigma_{i}(0), ..., \sigma_{i}(t)) = \sum_{\vec{\sigma}_{\partial i \setminus j}(0), ..., \vec{\sigma}_{\partial i \setminus j}(t)} \prod_{k \in \partial i \setminus j} m_{k \to i}(\sigma_{k}(0), ..., \sigma_{k}(t) | \sigma_{i}(0), ..., \sigma_{i}(t))$$

$$\prod_{s=1}^{t} \left[\frac{1}{N} \frac{e^{\beta h_{i}^{(j)}(s)\sigma_{i}(s)}}{2\cosh(\beta h_{i}^{(j)}(s))} + (1 - \frac{1}{N})\delta_{\sigma_{i}(s), \sigma_{i}(s-1)} \right] m_{i \to j}(\sigma_{i}(0))$$

The time factorized approximation :

$$m_{i \to j}(\sigma_{i}(t)) = \frac{1}{N} \sum_{\vec{\sigma}_{\partial i \setminus j}(t-1), \sigma_{i}(t-2)} \prod_{k \in \partial i \setminus j} m_{k \to i}(\sigma_{k}(t-1) | \sigma_{i}(t-2)) - \frac{e^{\beta h_{i}^{(j)}(t)\sigma_{i}(t)}}{2\cosh(\beta h_{i}^{(j)}(t))} m_{i \to j}(\sigma_{i}(t-2)) + (1 - \frac{1}{N}) \sum_{\sigma_{i}(t-1)} m_{i \to j}(\sigma_{i}(t-1)) \delta_{\sigma_{i}(t), \sigma_{i}(t-1)}$$

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Comparing dynamic cavity equations to Monte Carlo

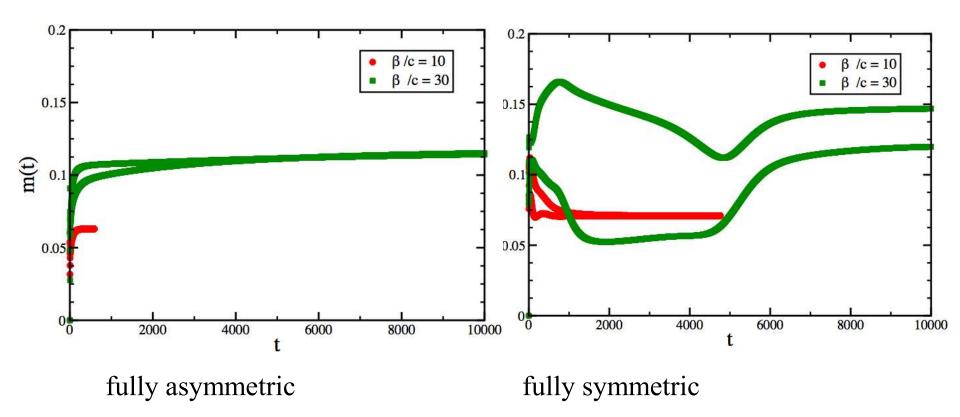
work in progress...

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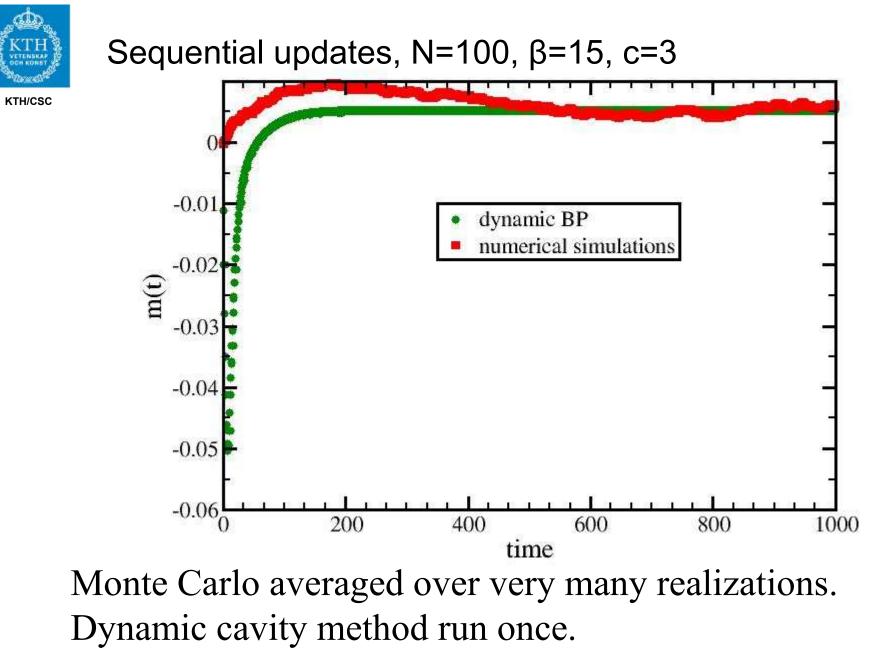
Parallel updates, different temperatures

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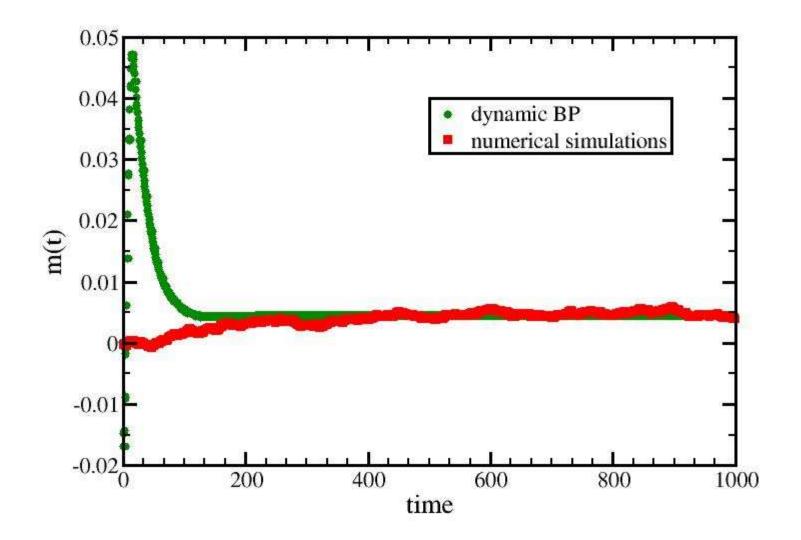
Average magnetization measured

 $m(t) = \frac{1}{N} \sum_{i=1}^{N} m_i(t)$



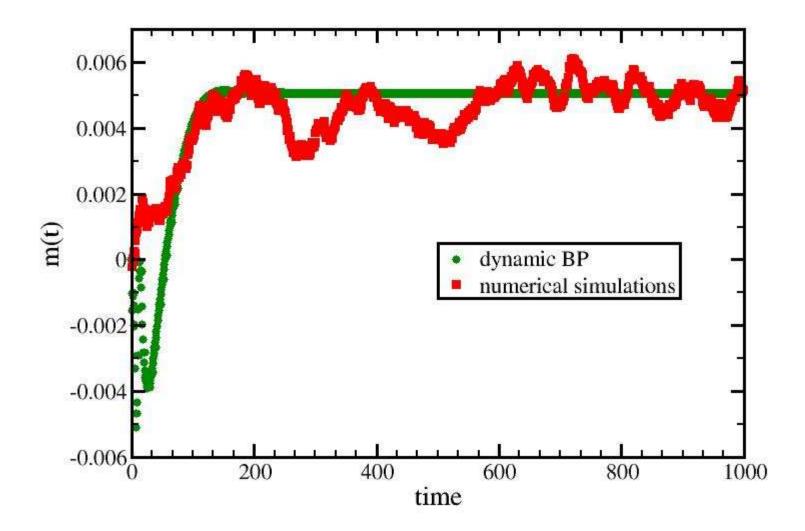


Some more sequential update cases....



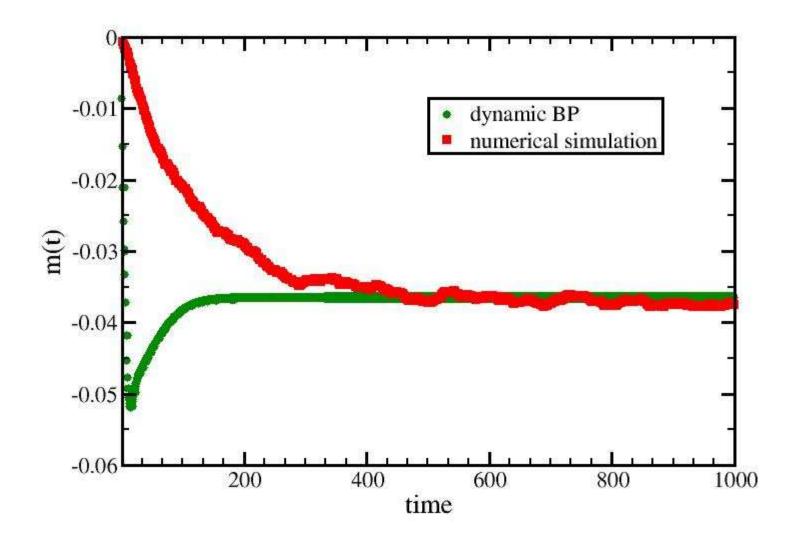


Yet some more sequential update cases....





And yet more still.





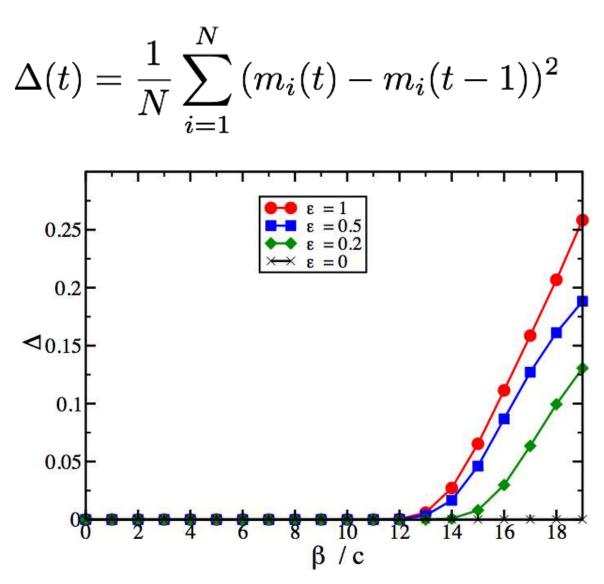
There seems to be something to it.

Therefore...to be continued...

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Parallel updates can have cyclic behaviour



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Thanks