

Multilevel methods for kernel interpolation in uncertainty quantification

Abi Srikumar

Joint work with Alec Gilbert, Mike Giles, Frances Kuo and Ian Sloan

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Introduction

What is **uncertainty quantification**?

We try to better understand models with intrinsic randomness to them.

We will look at **multilevel kernel-based lattice-point** approximation for PDE solutions with random coefficients where the diffusion coefficient is **periodic** in its stochastic variables.

Introduction

What is **uncertainty quantification**?

We try to better understand models with intrinsic randomness to them.

We will look at **multilevel kernel-based lattice-point** approximation for PDE solutions with random coefficients where the diffusion coefficient is **periodic** in its stochastic variables.

Note this is work in progress!!

Problem setting

Consider the stochastic PDE over bounded, convex domain $D \subset \mathbb{R}^d$,

$$\begin{aligned} -\nabla \cdot (a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) &= f(\mathbf{x}) & \mathbf{x} \in D, \\ u(\mathbf{x}, \mathbf{y}) &= 0, & \mathbf{x} \in \partial D, \end{aligned}$$

where $f \in L^2(D)$ is deterministic. Our random coefficient is now **periodic** in our stochastic variables,

$$a(\mathbf{x}, \mathbf{y}) = a_0(\mathbf{x}) + \sum_{j \geq 1} \sin(2\pi y_j) \psi_j(\mathbf{x})$$

where $y_j \sim \text{Unif}[-\frac{1}{2}, \frac{1}{2}]$ and $a_0, \psi_j \in L^\infty(D)$ for $j \geq 1$ such that $\sum_{j \geq 1} |\psi_j(\mathbf{x})| < \infty$ for any $\mathbf{x} \in D$.

Kaarnioja, Kuo and Sloan (2020)

Problem setting

Our assumptions

- 1 $a_0 \in L^\infty(D)$, $\psi_j \in L^\infty(D)$ for all $j \geq 1$ and $\sum_{j \geq 1} \|\psi_j\|_{L^\infty} < \infty$
- 2 $0 < a_{\min} \leq a(\mathbf{x}, \mathbf{y}) \leq a_{\max}$ for all $\mathbf{x} \in D$ and $\mathbf{y} \in \Omega$
- 3 $\sum_{j \geq 1} \|\psi_j\|_{L^\infty}^p < \infty$ for some $p \in (0, 1)$
- 4 $a_0 \in W^{1,\infty}(D)$ and $\sum_{j \geq 1} \|\psi_j\|_{W^{1,\infty}(D)} < \infty$ where $\|v\|_{W^{1,\infty}(D)} := \max\{\|v\|_{L^\infty}, \|\nabla v\|_{L^\infty}\}$
- 5 $\|\psi_1\|_{L^\infty} \geq \|\psi_2\|_{L^\infty(D)} \geq \dots$
- 6 D is a convex bounded polyhedron with plane faces

Kaarnioja, Kuo and Sloan (2020)

The plan

Considerations:

- Our field is infinite dimensional
- For approximation, we require the target function to be pointwise well-defined in both \mathbf{x} and \mathbf{y}
- Approximate the solution

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The plan

Considerations:

- Our field is infinite dimensional \rightarrow **Truncate the dimension**
- For approximation, we require the target function to be pointwise well-defined in both \mathbf{x} and \mathbf{y} \rightarrow **Finite element method**
- Approximate the solution

The plan

Considerations:

- Our field is infinite dimensional → **Truncate the dimension**
- For approximation, we require the target function to be pointwise well-defined in both \mathbf{x} and \mathbf{y} → **Finite element method**
- Approximate the solution → **Multilevel kernel interpolation**

The weighted Korobov space

We are interested in the Hilbert space $H_{\alpha,\gamma}$ of one-periodic L^2 functions with defined on $[0, 1]^s$ with absolutely convergent Fourier series.

The norm and inner product of $H_{\alpha,\gamma}$ are

$$\|f\|_{s,\alpha,\gamma}^2 := \sum_{\mathbf{h} \in \mathbb{Z}^s} |\widehat{f}(\mathbf{h})|^2 r_{\alpha,\gamma}(\mathbf{h}) \quad \text{and} \quad \langle f, g \rangle_{\alpha,\gamma} := \sum_{\mathbf{h} \in \mathbb{Z}^d} \widehat{f}(\mathbf{h}) \overline{\widehat{g}(\mathbf{h})} r_{\alpha,\gamma}(\mathbf{h}),$$

with

$$r_{\alpha,\gamma}(\mathbf{h}) := \frac{1}{\gamma_{\text{supp}(\mathbf{h})}} \prod_{j \in \text{supp}(\mathbf{h})} |h_j|^{2\alpha}.$$

For integer α , the norm can be written as

$$\|f\|_{H_{\alpha,\gamma}} = \sqrt{\sum_{\mathbf{u} \subseteq \{1:s\}} \frac{1}{(2\pi)^{2\alpha|\mathbf{u}|} \gamma_{\mathbf{u}}} \int_{[0,1]^{|\mathbf{u}|}} \left| \int_{[0,1]^{s-|\mathbf{u}|}} \left(\prod_{j \in \mathbf{u}} \frac{\partial^\alpha}{\partial y_j^\alpha} \right) f(\mathbf{y}) d\mathbf{y}_{-\mathbf{u}} \right|^2 d\mathbf{y}_{\mathbf{u}}}.$$

The weighted Korobov space

$H_{\alpha,\gamma}$ is a reproducing kernel Hilbert space with kernel

$$K(\mathbf{x}, \mathbf{y}) = \sum_{\mathbf{h} \in \mathbb{Z}^s} \frac{e^{2\pi \mathbf{h} \cdot (\mathbf{x} - \mathbf{y})}}{r_{\alpha,\gamma}(\mathbf{h})},$$

which satisfies

- 1 $K(\mathbf{x}, \mathbf{y}) = K(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}, \mathbf{y} \in [0, 1]^s$,
- 2 $K(\cdot, \mathbf{y}) \in H_{\alpha,\gamma}$ for all $\mathbf{y} \in [0, 1]^s$,
- 3 $\langle f, K(\cdot, \mathbf{y}) \rangle_{\alpha,\gamma} = f(\mathbf{y})$ for all $f \in H_{\alpha,\gamma}$ and all $\mathbf{y} \in [0, 1]^s$.

Rank-1 lattices

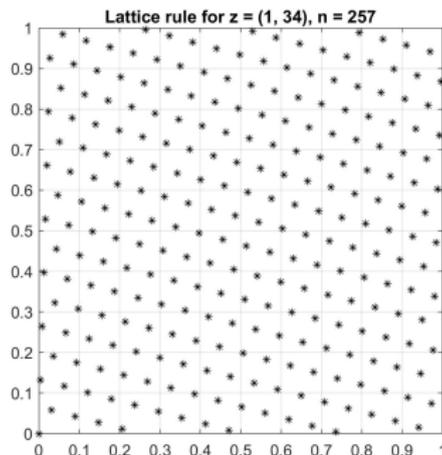
Lattice rules belong to *Quasi-Monte Carlo (QMC) methods*, cleverly designed integration techniques that are less susceptible to the curse of dimensionality.

An n -point rank-1 lattice is given by

$$\mathbf{t}_k = \frac{k\mathbf{z} \bmod n}{n} \quad \text{for } k = 0, \dots, n-1$$

where $\mathbf{z} \in \mathbb{U}_n^s$ is the generating vector.

The generating vector is constructed using a *component-by-component* algorithm.



Sloan and Joe (1994)

Lattice-based kernel approximation

We approximate $f \in H_{\alpha, \gamma}$ by the **kernel interpolant** of the form

$$I_n(f)(\mathbf{y}) := \sum_{k=0}^{n-1} a_k K(\mathbf{t}_k, \mathbf{y}) \quad \text{for } \mathbf{y} \in [0, 1]^s.$$

which interpolates f at n rank-1 lattice points.

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That is,

$$I_n(f)(\mathbf{t}_\ell) = f(\mathbf{t}_\ell) \quad \text{for all } \ell = 0, \dots, n-1.$$

The coefficients a_k are obtained by solving the resulting linear system,

$$f(\mathbf{t}_\ell) = \sum_{k=0}^{n-1} a_k K(\mathbf{t}_k, \mathbf{t}_\ell) \quad \text{for all } \ell = 0, \dots, n-1.$$

Note that:

- 1 Kernel interpolant is optimal for given function values.

Lattice-based kernel approximation

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Lattice-based kernel approximation

Note that:

- 1 Kernel interpolant is optimal for given function values.
- 2 Following from properties of the kernel and lattice structure, we have a circulant matrix \rightarrow fast Fourier Transform with cost $\mathcal{O}(n \log n)$
- 3 Aim is to construct the interpolant at a cheaper cost by leveraging multilevel methods

Multilevel methods

We want to estimate $\mathbb{E}[P]$, the easiest way is to take a direct average over a number of samples

$$\mathbb{E}[P] \approx \frac{1}{N} \sum_{n=1}^N P^{(n)}.$$

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Given a sequence P_0, \dots, P_{L-1} which approximates P_L with increasing accuracy, we have that

$$\mathbb{E}[P_L] = \mathbb{E}[P_0] + \sum_{\ell=1}^L \mathbb{E}[P_\ell - P_{\ell-1}].$$

This can be estimated by

$$\frac{1}{N_0} \sum_{n=1}^{N_0} P_0^{(0,n)} + \sum_{\ell=0}^L \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} (P_\ell^{(\ell,n)} - P_{\ell-1}^{(\ell,n)}).$$

- **Multilevel methods**

Giles (2008), Giles and Waterhouse (2009), Heinrich (1998), Heinrich (2001)

- **Uncertainty quantification**

Cliffe, Giles, Scheichl and Teckentrup (2011), Gilbert and Scheichl (2020), Hakula et al. (2023), Kaarnioja, Kuo and Sloan (2020), Kuo, Schwab and Sloan (2015)

- **Kernel-based approximation**

Belhadji, Bardenet and Chainais (2020), Kaarnioja et al. (2022), Schaback (1995), Schaback and Wendland (2006), Zeng, Kritzer and Hickernell (2009), Zeng, Leung and Hickernell (2006)

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Today: Theory for multilevel kernel interpolation !

Formulation of multilevel kernel interpolant

We begin by defining

$$u_\ell := u_{h_\ell}^{s_\ell}$$

as the finite element solution at level ℓ with mesh width h_ℓ and dimension truncated to s_ℓ .

We also use the notation $l_\ell := l_{n_\ell}$ to indicate the kernel interpolant constructed using n_ℓ lattice points.

Formulation of multilevel kernel interpolant

For $\ell = 0, 1, \dots$, consider a sequence of kernel interpolants I_ℓ using a decreasing number of points $n_0 > n_1 > \dots$ and a sequence of finite element approximations u_ℓ using an increasing number of finite element nodes, i.e., $h_0 > h_1 > \dots$.

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Now, the approximation at the maximum level $L \in \mathbb{N}$ is given by

$$I_L u_L := I_0 u_0 + \sum_{\ell=1}^L I_\ell (u_\ell - u_{\ell-1}).$$

Error breakdown

The total approximation error can be broken down as follows:

$$\begin{aligned}u - I_L u_L &= u - \sum_{\ell=0}^L I_\ell (u_\ell - u_{\ell-1}) \\&= u - u_{h_L}^{S_L} + \sum_{\ell=0}^L (I - I_\ell) (u_\ell - u_{\ell-1}) \\&= \underbrace{u - u^{S_L}}_{\text{DT error}} + \underbrace{u^{S_L} - u_{h_L}^{S_L}}_{\text{FE error}} + \underbrace{\sum_{\ell=0}^L (I - I_\ell) (u_\ell - u_{\ell-1})}_{\text{ML KI error}}\end{aligned}$$

Error breakdown

The total error can be expressed as

$$\begin{aligned} & \sqrt{\int_{\Omega} \int_D (u(\mathbf{x}, \mathbf{y}) - I_L u(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \\ & \leq \sqrt{\int_{\Omega} \int_D (u(\mathbf{x}, \mathbf{y}) - u^{sL}(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \\ & \quad + \sqrt{\int_{\Omega} \int_D (u^{sL}(\mathbf{x}, \mathbf{y}) - u_{h_L}^{sL}(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \\ & \quad + \sum_{\ell=0}^L \sqrt{\int_{\Omega} \int_D ((I - I_{\ell})(u_{\ell} - u_{\ell-1})(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \end{aligned}$$

Theorem (Kaarnioja et al. (2022))

Suppose the PDE problem satisfies the required conditions. Then for any $s \in \mathbb{N}$, there exists a constant $C > 0$ such that

$$\sqrt{\int_{\Omega} \int_D (u(\mathbf{x}, \mathbf{y}) - u^s(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \leq C s^{-\frac{1}{p} + \frac{1}{2}} \|f\|_{H^{-1}(D)},$$

where the constant $C > 0$ is independent of s and f .

Theorem (Kaarnioja et al. (2022))

Under the required assumptions, for every $\mathbf{y} \in \Omega$ and $f \in L^2(D)$, the following asymptotic convergence estimate holds

$$\|u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y})\|_{L^2(D)} \leq C h^2 \|f\|_{L^2(D)} \quad \text{as } h \rightarrow 0,$$

where the constant $C > 0$ is independent of h and \mathbf{y} .

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where the constant $C > 0$ is independent of h and \mathbf{y} .

Applying to dimension truncated problem, we have

$$\sqrt{\int_{\Omega} \int_D (u^s(\mathbf{x}, \mathbf{y}) - u_h^s(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \leq C h^2 \|f\|_{L^2(D)}.$$

Multilevel error

We now bound the Multilevel kernel interpolant component of error.

Recall $u_\ell = u_{h_\ell}^{s_\ell}$.

$$\begin{aligned} & \sum_{\ell=0}^L \sqrt{\int_{\Omega_\ell} \int_D ((I - I_\ell)(u_\ell - u_{\ell-1})(\mathbf{x}, \mathbf{y}))^2 d\mathbf{x} d\mathbf{y}} \\ &= \sqrt{\int_{\Omega_0} \int_D ((I - I_0)(u_0)(\mathbf{x}, \mathbf{y}))^2 d\mathbf{x} d\mathbf{y}} \\ & \quad + \sum_{\ell=1}^L \sqrt{\int_{\Omega_\ell} \int_D ((I - I_\ell)(u_\ell - u_{\ell-1})(\mathbf{x}, \mathbf{y}))^2 d\mathbf{x} d\mathbf{y}}, \end{aligned}$$

Kernel interpolation error

We define the worst-case error of approximation wrt the L^2 -norm as

$$e^{\text{wor}}(I_n, L_2) := \sup_{\|f\|_{H_{\alpha, \gamma}} < 1} \|f - I_n(f)\|_{L^2}.$$

Kernel interpolation error

We define the worst-case error of approximation wrt the L^2 -norm as

$$e^{\text{wor}}(I_n, L_2) := \sup_{\|f\|_{H_{\alpha, \gamma}} < 1} \|f - I_n(f)\|_{L^2}.$$

Following from the **optimality of the kernel interpolant**, we have

$$e^{\text{wor}}(I_n, L_2) \leq \mathcal{S}_n(\mathbf{z}).$$

$\mathcal{S}_n(\mathbf{z})$ (which bounds the trig polynomial approximation) is shown in Cools, Kuo, Nuyens and Sloan (2021) and Kuo, Mo and Nuyens (2023+) to have convergence $\mathcal{O}(n^{-\alpha/2+\delta})$ for $\delta > 0$.

Theorem (Kaarnioja et al. (2022))

Given $s \geq 1$, $\alpha > 1/2$ and weights $\gamma = (\gamma_u)_{u \in \mathbb{N}}$, a lattice-based kernel interpolant I_n can be constructed such that

$$e^{\text{wor}}(I_n, L_2) \leq C_{\gamma, \delta} n^{-\frac{\alpha}{2} + \delta} \quad \text{for all } \delta \in (0, \alpha/2)$$

where the implied constant depends on α but is independent of s .

Multilevel error

Now, considering a term in the multilevel error component,

$$\begin{aligned} & \sqrt{\int_{\Omega_\ell} \int_D ((I - I_\ell)(u_\ell - u_{\ell-1})(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \\ & \leq \sqrt{\int_D \int_{\Omega_\ell} ((I - I_\ell)(u_\ell - u_{\ell-1})(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{y} \, d\mathbf{x}} \\ & \leq \sqrt{\int_D \|(I - I_\ell)(u_\ell - u_{\ell-1})(\mathbf{x}, \cdot)\|_{L^2(\Omega_\ell)}^2 \, d\mathbf{x}} \\ & \leq e^{\text{wor}}(I_\ell, L^2(\Omega_\ell)) \sqrt{\int_D \|(u_\ell - u_{\ell-1})(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega_\ell)}^2 \, d\mathbf{x}} \end{aligned}$$

Multilevel error

$$\begin{aligned} & e^{\text{wor}}(I_\ell, L^2(\Omega_\ell)) \sqrt{\int_D \|(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega_\ell)}^2 d\mathbf{x}} \\ & \leq e^{\text{wor}}(I_\ell, L^2(\Omega_\ell)) \left[\sqrt{\int_D \|(u_{h_{\ell-1}}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega_\ell)}^2 d\mathbf{x}} \right. \\ & \quad \left. + \sqrt{\int_D \|(u^{s_\ell} - u_{h_\ell}^{s_\ell})(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega_\ell)}^2 d\mathbf{x}} + \sqrt{\int_D \|(u^{s_\ell} - u_{h_{\ell-1}}^{s_\ell})(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega_\ell)}^2 d\mathbf{x}} \right] \end{aligned}$$

Multilevel error

Multilevel DT error

Theorem (Gilbert, Giles, Kuo, Sloan and S. (In prep.))

Suppose the PDE problem satisfies the required assumptions. For $\alpha \geq 1$, $f \in L^2(D)$ and $b_i := \frac{\|\psi_j\|_{L^\infty}}{a_{\min}}$, the weight parameters $(\gamma_u)_{u \subset \mathbb{N}}$ can be chosen such that

$$\begin{aligned} & \sqrt{\int_D \|(u_h^{s_\ell} - u_h^{s_{\ell-1}})(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega_\ell)}^2 d\mathbf{x}} \\ & \leq \frac{C \|f\|_{H^{-1}(D)}}{s^{\min(\frac{1}{p}-1, \eta)}} \sqrt{\sum_{u \subseteq \{1:s_\ell\}} \frac{1}{\gamma_u} \left(\sum_{\mathbf{m} \in \{1:\alpha\}^{|u|}} (|\mathbf{m}| + k)! \prod_{i \in u} b_i^{m_i} S(\alpha, m_i) \right)^2}, \end{aligned}$$

where $\eta > 0$, $k \geq \alpha$ and $C > 0$ is independent of s_ℓ and $s_{\ell-1}$.

Multilevel error

Multilevel FE error

Theorem (Gilbert, Giles, Kuo, Sloan and S. (In prep.))

Suppose the PDE problem satisfies the required assumptions. For $\alpha \geq 1$, weight parameters $(\gamma_u)_{u \subset \mathbb{N}}$, $f \in L^2(D)$ and defining $\bar{b}_i := \frac{\|\nabla \psi_j\|_{L^\infty}}{a_{\min}}$, the following estimate holds

$$\begin{aligned} & \sqrt{\int_D \|(u^s - u_h^s)(\mathbf{x}, \cdot)\|_{H_{\alpha, \gamma}(\Omega)}^2 d\mathbf{x}} \\ & \leq C h^2 \|f\|_{L^2(D)} \sqrt{\sum_{u \subseteq \{1:s\}} \frac{1}{\gamma_u} \left(\sum_{\mathbf{m} \in \{1:\alpha\}^{|u|}} (|\mathbf{m}| + 5)! \prod_{i \in u} \bar{b}_i^{m_i} S(\alpha, m_i) \right)^2}, \end{aligned}$$

where $C > 0$ is independent of h .

Multilevel error

Multilevel FE error

Sketch of the proof:

- 1 Cauchy-Schwarz and Fubini's theorem
- 2 We need bounds for $\|\partial^\nu(u - u_h)(\cdot, \mathbf{y})\|_{L^2(D)}$
- 3 **Theorem.**

$$\|\partial^\nu(u - u_h)\|_{H_0^1(D)} \leq C h \|f\|_{L^2} (2\pi)^{|\nu|} \sum_{\mathbf{m} \leq \nu} (|\mathbf{m}| + 2)! \bar{\mathbf{b}}^{\mathbf{m}} \prod_{i \geq 1} S(\nu_i, m_i)$$

- 4 Aubin-Nitsche duality argument
- 5 **Theorem.**

$$\|\partial^\nu(u - u_h)\|_{L^2(D)} \leq C h^2 \|f\|_{L^2} (2\pi)^{|\nu|} \sum_{\mathbf{m} \leq \nu} (|\mathbf{m}| + 5)! \bar{\mathbf{b}}^{\mathbf{m}} \prod_{i \geq 1} S(\nu_i, m_i)$$

Putting it together

Error \approx DT error + FE error + ML KI error

Theorem (Gilbert, Giles, Kuo, Sloan and S. (In prep.))

Suppose the PDE problem satisfies the required assumptions. For $\alpha \geq 1$, and $f \in L^2(D)$, the weight parameters $(\gamma_u)_{u \in \mathbb{N}}$ can be chosen such that

$$\begin{aligned} & \sqrt{\int_{\Omega} \int_D (u(\mathbf{x}, \mathbf{y}) - I_L u(\mathbf{x}, \mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y}} \\ & \leq C_{\text{params}} \left(s_L^{-\frac{1}{p} + \frac{1}{2}} + h_L^2 + \sum_{\ell=0}^L \frac{1}{n_{\ell}^{\frac{\alpha}{2} - \delta}} (h_{\ell-1}^2 + s_{\ell-1}^{-\min(\frac{1}{p} - 1, \eta)}) \right) \end{aligned}$$

TBA.

Conclusion

We construct a multilevel kernel interpolant in the hope of reducing the current cost.

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To do

- Full implementation and numerics of multilevel methodology
- Possibly improve multilevel dimension truncation error
- Multilevel approximation for other applications

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Thank you for your attention :)

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