Ensemble propagation for efficient uncertainty quantification on emerging architectures: Application to thermomechanical contact

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Objective

Efficient sampling-based uncertainty quantification with multiphysics models on emerging architectures.

Emerging architectures

Vectorization (Single Instruction Multiple Data) and **efficient memory usage** for optimal performance

	2.1	-8.	5.7	49.	0.	3.9	0.1	0.9
×	5.	-2.2	0.	0.01	100.	3.9	0.1	-0.9
=	10.5	17.6	0.	0.49	0.	15.21	0.01	-0.81

Fig. 1. Vectorial multiplication of 8 doubles on Xeon Phi.

On Xeon Phi KNL, the maximum speed up is 244 and 1952 without and with double vectorization respectively.

Sampling-based uncertainty quantification (UQ)

The Monte Carlo method is well-adapted to problems of uncertainty quantification:

- with nonsmooth responses,
- in very high dimension.

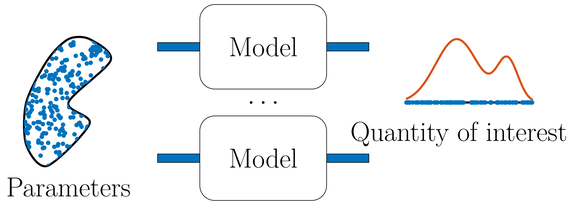

Fig. 2. Sampling-based UQ.

Ensemble propagation

Instead of individually evaluating each instance of the model, ensemble propagation (EP) [1] consists in simultaneously evaluating a subset of samples of the model.

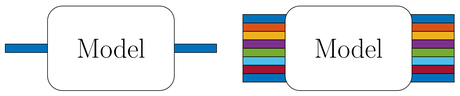

Fig. 3. Sample and ensemble propagation with 8 samples.

EP has the following advantages:

- Improved probability of auto-vectorization,
- Improved memory usage,
- Reuse of common variables,
- Reduction of Message Passing Interface (MPI) latency per sample.

Advantage: EP can improve the performance of sampling-based UQ on emerging architectures.

EP raises new challenges:

- Increased memory usage,
- Code divergence.

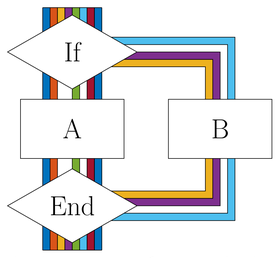

Fig. 4. Code divergence of a sample dependent If.

Challenge: Code divergence inside an ensemble may reduce the computational performance.

Trilinos

Such an embedded EP is currently being implemented based on the use of C++ templating in Stokhos, a software component of Trilinos [2].

ITER spectroscope

One of the possible options of the first mirror of the CXRS ITER spectroscope [3] will be bolted to a holder which will cool the mirror heated by the plasma. The deformation of the mirror surface depends on the temperature, which itself depends on the contact status of the bolts.

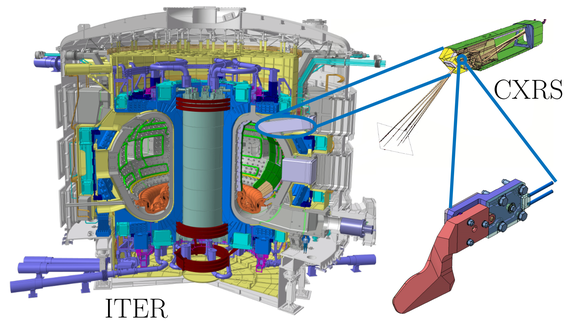

Fig. 5. CXRS ITER spectroscope and its first mirror.

Contact

Contact constraints can be either **active** or **inactive**.

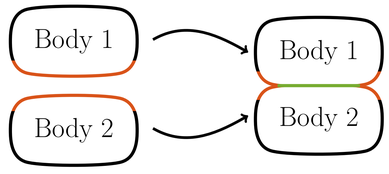

Fig. 6. Contact local status.

The active and inactive constraints are not known a priori and may modify the graph of the discretized problem.

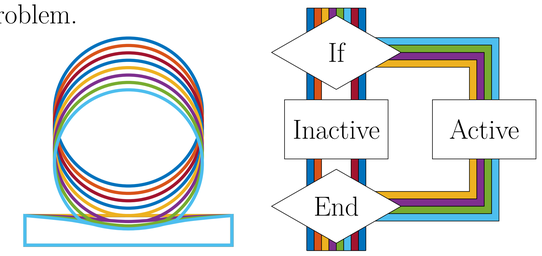

Fig. 7. Sampling dependent contact status.

Ongoing study

- How to solve the model efficiently for any given ensemble of sufficiently similar samples?
  - Select the most appropriate contact formulation for EP,
  - Select the most appropriate Krylov solver adequate for contact with EP,
  - Suppress the code divergences using sample independent criteria and using masking.

Fig. 8. Masking of the If condition of Fig. 4 using mask m.

- How to group sufficiently similar samples in the same ensemble?
  - Grouping samples according to their predicted contact status,
  - Grouping samples according to their estimated number of linear iterations of Krylov method.

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