Distributed parameter states in QUESO

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1 Introduction

This document describes the current, serial, state of the parameter vector in `QUESO` and makes a plan to transition to a distributed state.

1.1 The current state

The current state of the parameter vector in `QUESO` is serial. Parallelism in `QUESO` presents itself in two ways: 1) independent parallel Markov chains that execute concurrently; and 2) a mechanism, an MPI communicator, that `QUESO` creates as part of the construction of `FullEnvironment` the user can hand to a forward problem demanding parallelism. Neither of these parallel capabilities distribute the parameter vector across multiple processes. In other words, each chain's process holds exactly the same parameter vector value in the likelihood.

Here is some example commented code that executes the current situation:

```
#include <queso/Environment.h>
#include <queso/GslVector.h>
#include <queso/GslMatrix.h>
#include <queso/ScalarFunction.h>
#include <queso/VectorSpace.h>
#include <queso/BoxSubset.h>

using namespace QUESO;

template <class V = GslVector, class M = GslMatrix>
class Likelihood : public BaseScalarFunction<V, M>
{
public:
  Likelihood(const char * prefix,
             const VectorSet<V, M> & domainSet)
    : BaseScalarFunction<V, M>(prefix, domainSet),
      m_env(domainSet.env())
  {
  }

  virtual double lnValue(const V & param) const
  {
    if (m_env.subRank() == 0) {
      std::cout << "Rank 0 param: " << param << '\n';
    }
    else {  // Rank 1
      std::cout << "Rank 1 param: " << param << '\n';
    }

    return 1.0;
  }

  virtual double actualValue(const V&, const V*, V*,
                             M*, V*) const
  {
    return 1.0;
  }

  const BaseEnvironment & m_env;
};
```

```
int main(int argc, char ** argv)
{
  // We'll assume the program was executed with
  // mpirun -np 2 and there's only one chain.

  MPI_Init(&argc, &argv);
  FullEnvironment env(MPI_COMM_WORLD, argv[1], "",
                      NULL);
  VectorSpace<> paramSpace(env, "", 2, NULL);
  GslVector min(paramSpace.zeroVector());
  GslVector max(paramSpace.zeroVector());
  min[0] = 0.0;
  min[1] = 0.0;
  max[0] = 1.0;
  max[1] = 1.0;
  BoxSubset<> paramDomain("", paramSpace, min, max);
  Likelihood<> likelihood("", paramDomain);

  GslVector point(paramSpace.zeroVector());
  point[0] = 0.5;
  point[1] = 0.5;
  likelihood.lnValue(point);  // Both ranks print the
                              // same parameter value

  MPI_Finalize();
  return 0;
}
```

1.2 Why we need a distributed state

There are some issues with a serial parameter vector, and some benefits to moving to a distributed parameter vector.

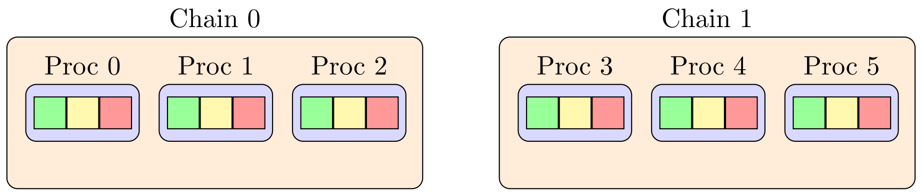
- There are problems with large parameter vectors (discretized fields) that necessitate distribution across multiple processes;
- Parallel parameter vector means `QUESO` can leverage existing high performance linear algebra packages for better compute resource usage;
- High performance linear algebra packages provide better performing optimization algorithms we could use before sampling;
- The serial implementation requires GSL, and GSL is licensed under the GPL. We have customers at the labs that would like to ship `QUESO` as a binary and GPL third-party libraries prevent this from happening.

– A rebuttal to this point might be to use an alternative serial implementation with a more liberal license. This is a reasonable suggestion but it doesn't address the first three points.

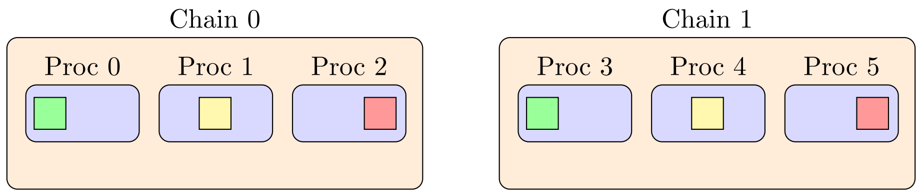
2 How the future might look

2.1 Parameter distribution in parallel

If the user requests multiple processes per chain, then an approach we might take is to distribute the parameter across those processes. In the code example above, that would mean process 0 sees only the first element of `point` and process 1 sees only the second element. Here's a depiction before the change:



And here's what it looks like after the change:



To maintain compatibility with existing parallel forward problems, `QUESO` will do all the necessary communication before a likelihood call to organise the parameter vector. Inside the likelihood each process belonging to the chain communicator will receive a serial version of the parameter vector. Every process will hold an exact copy of the parameter vector.

The user will not be burdened with providing the mechanism needed to pass a distributed parameter vector to their forward model. Therefore, parallel forward codes that worked with a serial parameter vector will still continue to work when `QUESO` distributes the parameter vector representation internally.

What about the case where the user needs multiple independent model evaluations for a single likelihood calculation? This case arises when there are multiple experimental data points. It is reasonable to leverage independent concurrency for these data points. Internally, the parameter vector will be distributed over all processes belonging to the chain communicator. `QUESO` is not concerned with how these processes are leveraged by the application that executes the forward model. For example, if three process are needed for a single model evaluation and two model evaluations are needed for a single likelihood evaluation then `QUESO` will distribute the parameter vector over all six processes. `QUESO` will do all the necessary MPI communcation before a likelihood call to ensure that every process belonging to a chain communicator holds the entire parameter vector.

2.2 Memory and usability considerations

We noted in the previous subsection that the parameter vector is distributed across the processes involved in a chain communicator.

2.2.1 Usability

Once a model evaluation needs to be done, it is reasonable to expect that the model communicator needs the entire parameter vector. If the parameter vector is distributed across the entire chain communicator after a call to the likelihood, the user would be burdened with the point-to-point communication required to organise the parameter vector for their model, or their model must be written in such a way that understands and respects `QUESO`'s choice of how to distributed the parameter vector among the processes in the chain communicator. This introduces a rather large barrier to entry.

Making each process hold the entire parameter vector (inside the likelihood) offers a much more user-friendly experience; the user needn't concern themselves with a potentially burdensome and tricky point-to-point communication and bookkeeping. It also offers the possibility of allowing older forward codes to work with `QUESO` since no code changes would be needed.

2.2.2 Memory

It is clear that more memory is required if each process in the chain communicator holds a copy of the entire parameter vector. It doesn't seem too detrimental, however.

In the worst case the user intends to solve an inverse problem in function space. In other words, the parameter vector represents a discretised field and this discretisation may be quite fine. For inverse problems on function space, one typically represents the random field by, for example, a truncated KL expansion. Inference is done on the coefficients in this expansion. It is uncommon to execute an inference at every length scale the discretisation can represent. In other words, the inference is done a number of KL coefficients that is typically much smaller than the number of degrees of freedom offered by the choice of discretisation.

2.3 From the user's perspective

There are a few things to look at:

1. The parameter space
2. The parameter domain
3. Distributions on the domain (priors)
4. Interacting with vectors and matrices
5. The likelihood

These should change as little as possible.

2.3.1 The parameter space

At present, the user calls the following to instantiate a parameter space of dimension 2,

```
MPI_Init(&argc, &argv);
FullEnvironment env(MPI_COMM_WORLD, argv[1], "",
                    NULL);
VectorSpace<> paramSpace(env, "", 2, NULL);
```

The parameter space is the same for each chain. It is only *within* a chain that the parameter is paritioned. There is a clear constraint here; the number of processes belonging to the chain must divide the dimension of the parameter space. This might be problematic in the situation where the forward model needs 10 processes to run quickly for a likelihood evaluation but the user can't ask for more than 2 processes.

Can we avoid this constraint? Maybe we allow the user to ask for more processes per chain and just use a subset of them. For example, if the user asks for 10 processes per chain for the forward model evaluation then `QUESO` would also ask for how many of those the parameter should be distributed over.

2.3.2 The parameter domain

For a `BoxSubset`, which is the most common domain, the user calls

```
BoxSubset<> paramDomain("", paramSpace, min, max);
```

The parameter space is already partitioned and `min` and `max` belong to the parameter space. Everything is already set up for the parameter domain and nothing needs to be done here from the user's perspective.

What about other domains? Another common domain is the `ConcatenatedSubset` . What about user-defined domains?

2.3.3 Distributions on partitioned domains

As an example, a user might construct a Gaussian distribution for the prior. The user calls

```
GaussianVectorRV<> prior("", paramDomain, mean,
                         covariance);
```

From the user's perspective, nothing would need to change. The mean belongs to the already-partitioned parameter vector space, and so does the covariance matrix.

Any distributions that rely on vectors or matrices for construction will lie in the already-partitioned space and the user will see no changes in their statistical application.

2.3.4 Interacting with vectors and matrices

We mentioned briefly that nothing special needs to be done to set up vector spaces and domains. We saw that these may depends on vectors and matrices the user must construct, and we explore that interaction here.

The user may interact with vectors in two different ways: 1) the user interacts with a serial vector; or 2) the user interacts with a parallel vector. The dimension of the vector space (integer passed in the `VectorSpace<>` constructor) is the global dimension. This is important to note, because `QUESO` will use it to determine which of the two interactions are used. If the serial vector interaction is used, then the length of each local vector is exactly the same as the global dimension. If the parallel vector interaction is used, then the sum of each of the local vector lengths is equal to the global dimension. If the user chooses to interact with a parallel vector then they are explicitly defining a partioning of that vector among processes in the chain communicator. `QUESO` will respect this partioning when doing, for example, matrix-vector operations. If the user interacts with a serial vector then `QUESO` will parition it automatically before doing matrix-vector operations. This code

```
// Serial vector interaction
GslVector<> v(paramSpace.zeroVector());
v[0] = 1.0;
v[1] = 2.0;
```

will set global (and local) index 0 on process 0 and global (and local) index 0 on prcoessor 1. Both processes belonging to the chain hold the 2-vector $(1, 2)$. This code

```
// Parallel vector interaction
Map map(2, 0, env.subComm());
GslVector<> v(env, map);

if (env.subRank() == 0) {
  v[0] = 1.0;
}
else if (env.subRank() == 1) {
  v[0] = 2.0;
}
```

will set local index 0 on process 0 and local index 0 on process 1. Local index 0 on processor 1 should map to global index 1 for `v`. Process 0 holds the 1-vector (1) and process 1 holds the 1-vector (2). Together they represent the partitioned 2-vector $(1, 2)$.

Interacting with matrices has a similar story. The user can interact with a serial matrix and `QUESO` will partition it behind the scences, or the user can choose a partitioning and `QUESO` will respect the user's choice. This code

```
// Parallel matrix interaction
GslMatrix<> A(env, map, 2);

if (env.subRank() == 0) {
  A(0, 0) = 1.0;
  A(0, 1) = 0.5;
}
else if (env.subRank() == 1) {
  A(0, 0) = 0.5;
  A(0, 1) = 1.0;
}
```

will set local row index 0 on process 0 and local row index 0 on process 1. Local row index 0 on process 1 should map to global row index 1 for `A`.

2.3.5 The likelihood

This part, from the user's perspective, doesn't change. Inside the call to `lnValue` the parameter `param` (from the first code example) doesn't change. It is a serial vector; each process belonging to the chain communicator has an exact copy of the global vector `param`.