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A Reimplementation of the Finite Element Method Software Package using FLENS

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Introduction

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  2. Replace linear algebra operations with BLAS equivalents.
  3. Offer two versions of solvers, one using BLAS notation, one using overloaded operators.

Replacing data storage objects

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- Some objects can be directly converted:

$$\begin{aligned} \texttt{Vector} &\rightarrow \texttt{DenseVector}\langle\texttt{Array}\langle\texttt{double}\rangle\ \rangle \\ \texttt{IndexVector} &\rightarrow \texttt{DenseVector}\langle\texttt{Array}\langle\texttt{int}\rangle\ \rangle \end{aligned}$$

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- FLENS offers a CRS matrix implementation, but it must be initialised from a sparse matrix using the coordinate storage scheme.

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  ↪ Derived from a FLENS `DenseVector`:

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1 template <typename VTYPE = FLvNonMPI>
2 struct FLENSDataVector
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  - ↪ Contains almost all objects and methods from the `DataVector`:

```
1 const Coupling &coupling;
2
3 void typeII_2_I();
4 void typeI_2_II();
5
6 void commCrossPoints();
7 void commBoundaryNodes();
```

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  - ↪ More rigorous.
  - ↪ Makes many assertions redundant, as all type checking is done at compile time.

BLAS and the Conjugate Gradient solver

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  - ↪ Available via overloaded operators in FLENS.
- GotoBLAS / OpenBLAS / ATLAS
  - ↪ Basically 'supercharged' BLAS routines, usually optimised for a specific processor.
  - ↪ Can be linked into FLENS (to replace FLENS BLAS routines) trivially (one compiler flag + linker paths).

BLAS

- FEM Package function call:

```
1 CRSmatVec(p,A,x);
2 add(r2,p,-1.);
```

BLAS

- Our function call via BLAS:

```
1 blas::mv(NoTrans, 1., A, x, 0., p);
2 blas::axpy(-1., p, r2);
```

BLAS

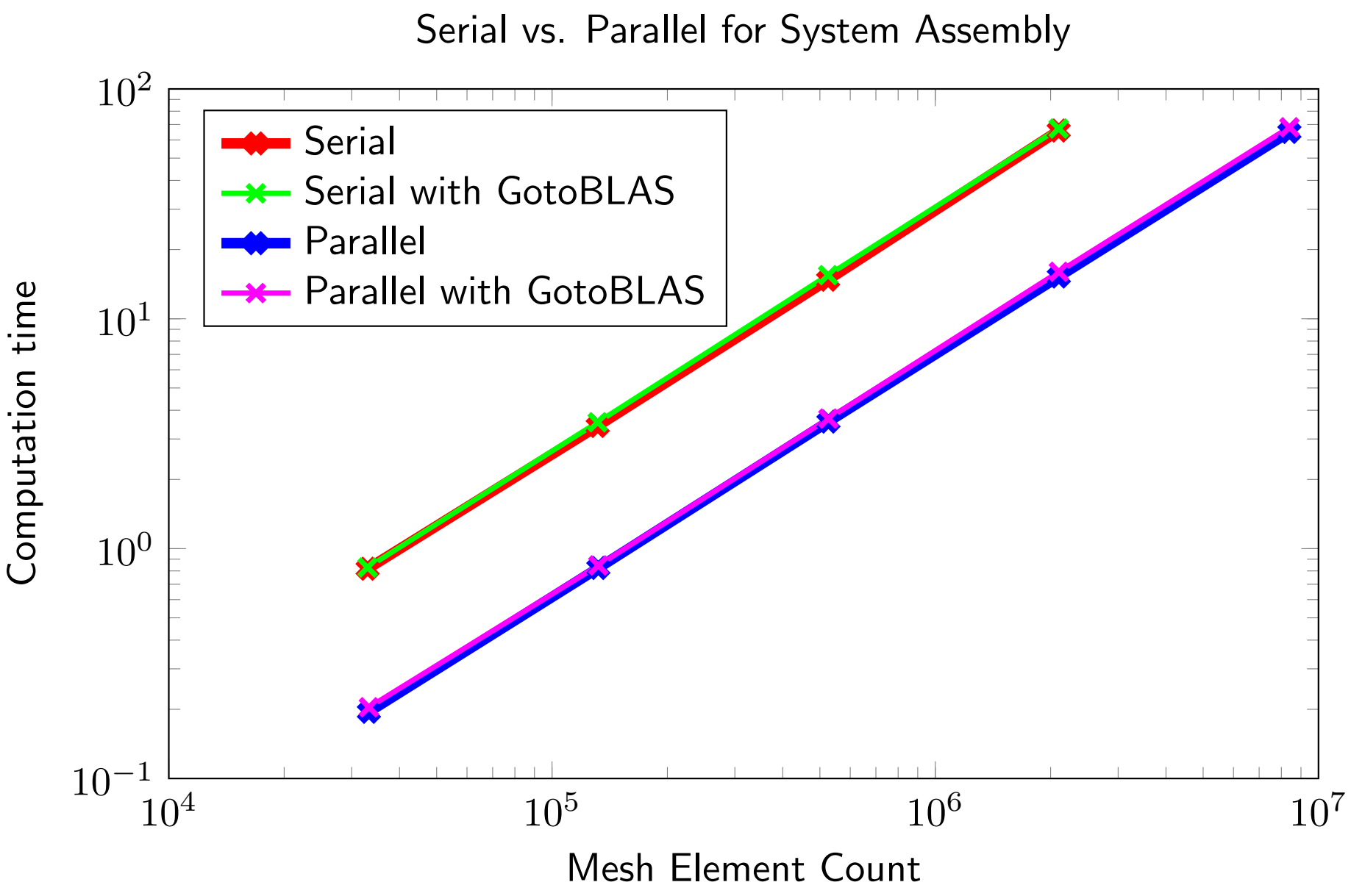
- Our function call via overloaded operators:

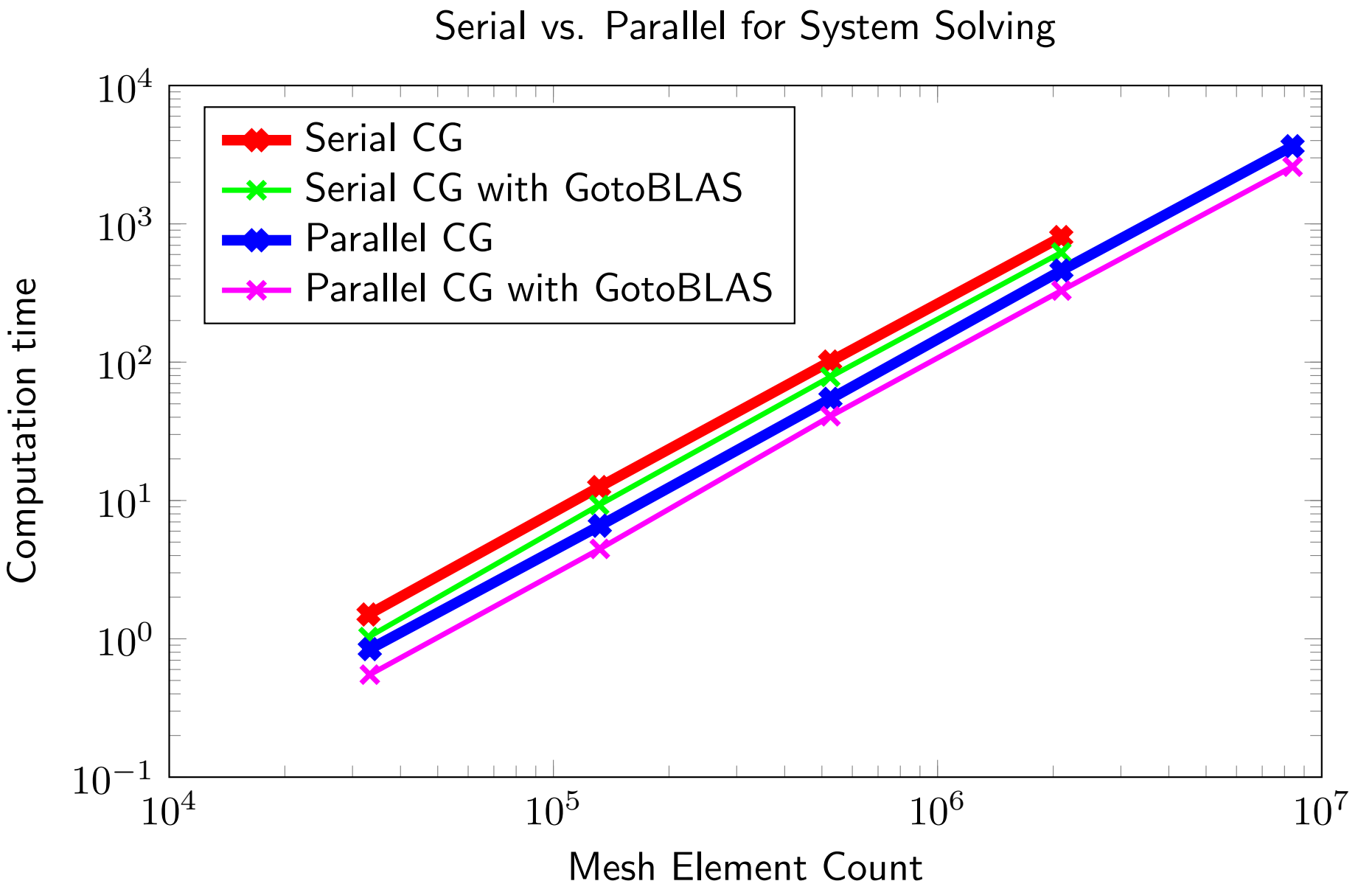
```
1 p = A*x;
2 r2 = r2 - p;
```

BLAS

- Care was taken when overloading BLAS operations that require MPI communications:

```
1  //Overloaded dot - performs appropriate communication:
2  double
3  dot(const FLENSDataVector<FLvTypeI> &x1,
4      const FLENSDataVector<FLvTypeII> &x2)
5  {
6    //Upcast to DenseVector, and use the standard blas::dot:
7    double value =
8        blas::dot(
9          *static_cast<const DenseVector<Array<double> > *>(&x1),
10         *static_cast<const DenseVector<Array<double> > *>(&x2)
11       );
12
13   double v = 0;
14   //*** Communication to add values from other processes ***/
15   MPI::COMM_WORLD.Allreduce(&value,&v,1,MPI::DOUBLE,MPI::SUM);
16
17   return v;
18 }
```


Serial vs. Parallel for System Assembly
Serial
Serial with GotoBLAS
Parallel
Parallel with GotoBLAS
Computation time
Mesh Element Count
10^2
10^1
10^0
10^{-1}
10^4
10^5
10^6
10^7


Serial vs. Parallel for System Solving
Serial CG
Serial CG with GotoBLAS
Parallel CG
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Computation time
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10^{4}
10^{3}
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10^{4}
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10^{6}
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The End