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Parallel Design Pattern for Computational Biology and Scientific Computing

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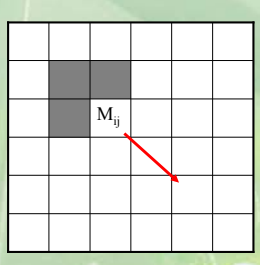
1. Abstract

Dynamic programming is an important algorithm design technique in computational biology and scientific computing. Typical applications using this technique are very computing-intensive and suffer from long runtimes on sequential architectures. Parallel program design patterns provide a new tool to semi automatically generate parallel programs. In this paper we present a new parallel pattern called the "block-cyclic based wavefront" to parallelize typical dynamic programming algorithms in computational biology and scientific computing. We show how this technique leads to significant run-time savings on PC clusters.

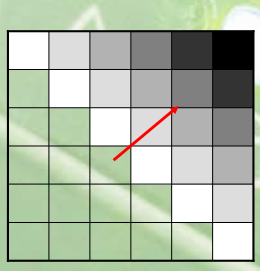
2. Dynamic Programming Algorithm : Regular and Irregular Wavefront Computation

$$M(i,j) = \max \begin{cases} M(i-1,j-1) + s(Ai, Bj), \\ M(i-1,j)-d, \\ M(i,j-1)-d, \\ 0; \end{cases}$$

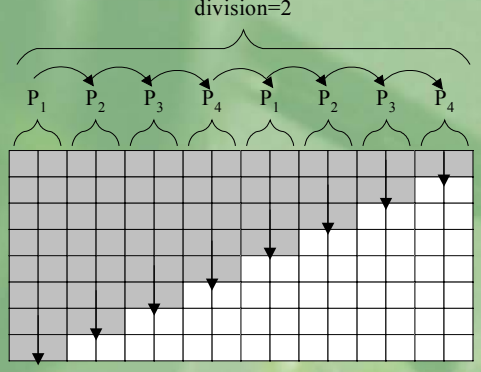


$$M(i,j) = \max \begin{cases} M(i+1,j-1) + \delta(i,j), \\ M(i,j-1), \\ M(i+1,j), \\ \max_{i<k<j}[M(i,k)+M(k+1,j)]; \end{cases}$$

where $i < j$



3. Block-Cyclic Based Partition for Distributed Memory Parallel Computers

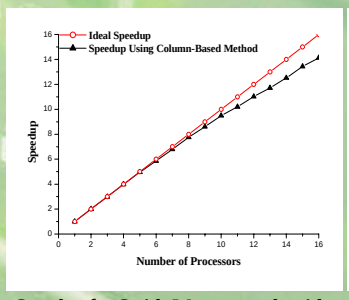


- The parameter *division* is used to implement a cyclic distribution of columns to processors.

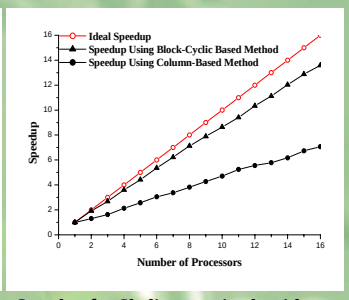
4. Implementation

```
template <class datatype>
class Wavefront{
public:
/* The constructor method uses the user-specified parameters to initialize the framework */
        Wavefront (int my_rank, int  processornumber, int matrixwidth, int matrixheight,
                   int division, int blocksize);
        void launch (){
                preprocess ();
                commonpreprocess();
                while (the division loop is not completed){
                        processor 1{
                                prepare1 ();
                                commonprepare1();
                                operate1 ();
                        }
                        processor 2 to P{
                                prepareP ();
                                commonprepareP();
                                operateP();
                        }
                }
                postprocess ();
        }
/* These three methods are used to implement the block-cyclic distribution scheme */
        void commonpreprocess(){};
        void commonprepare1(){};
        void commonprepareP(){};
/* These four methods allow users to specify customized behavior for a given application */
        virtual void preprocess (){};
        virtual void postprocess (){};
        virtual void prepare1 (){};
        virtual void prepareP (){};
/* These two methods are used to implement the compute-communicate procedure */
        virtual void operate1 (){};
        virtual void operateP (){};
/* This method is provided by the user to compute the node (i, j), it is called by the
   methods operate1() and operateP() */
        virtual void application (){};
};
```

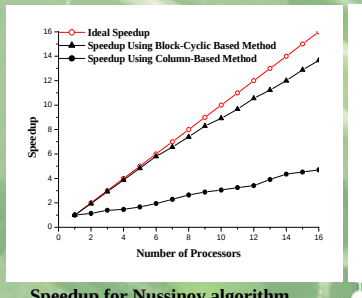
5. Results



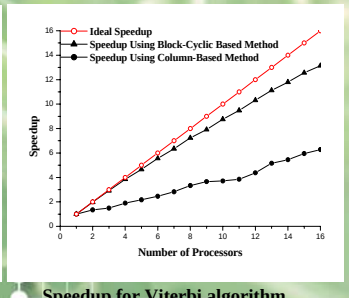
Speedup for Smith-Waterman algorithm



Speedup for Skyline matrix algorithm



Speedup for Nussinov algorithm



Speedup for Viterbi algorithm

6. Conclusions

- Semi-automatic generation of parallel programs
- Substantial performance gains for irregular dynamic programming applications