Using Co-Array Fortran to Enhance the Scalability of the EPIC Code

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Outline

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Project Description

- Investigate benefits of CAF
  - Replace MPI with CAF in key regions
- Begin to establish CAF ‘Best Practice’
- Improve EPIC performance for user base

CAF Overview

In a nutshell, CAF replaces this:

```
CALL MPI_SEND(A,N,MPI_REAL,MYPE+M,TAG, COMM,IERR)
CALL MPI_RECV(A,N,MPI_REAL,MYPE-M,TAG, COMM,ISTAT,IERR)
```

with this:

```
A(1:N)[MYPE+M]=A(1:N)
```

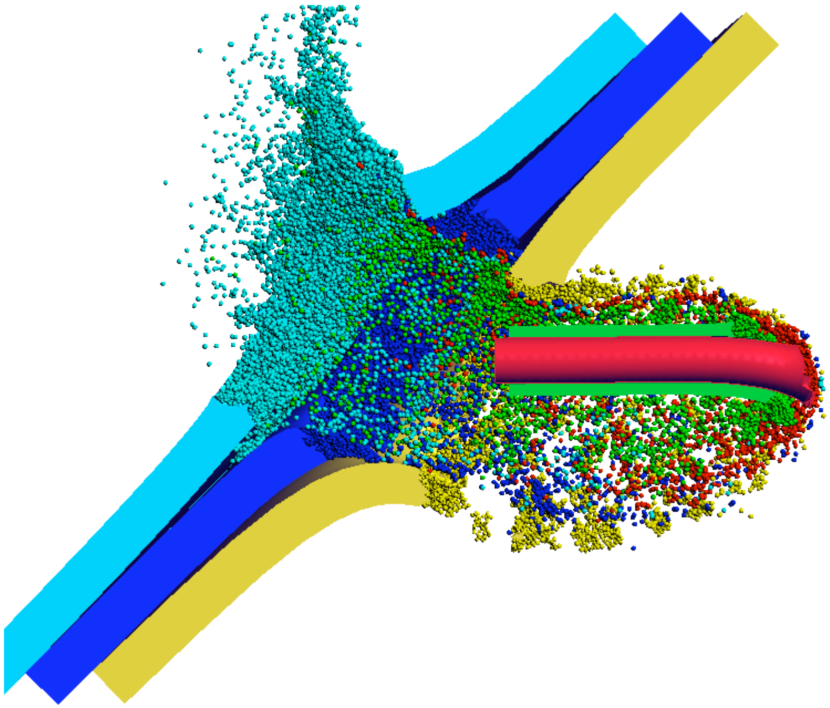
- **Both code fragments move N elements of A from CPU MYPE to CPU MYPE+M**
- **The CAF code is:**
  - **Actual language syntax, rather than library calls**
  - ***One-sided*, so that only one CPU needs to execute code for data to be communicated**
- **CAF on the X1E is *native***
  - **Hardware instructions directly load/store remote data**

Advantages of CAF

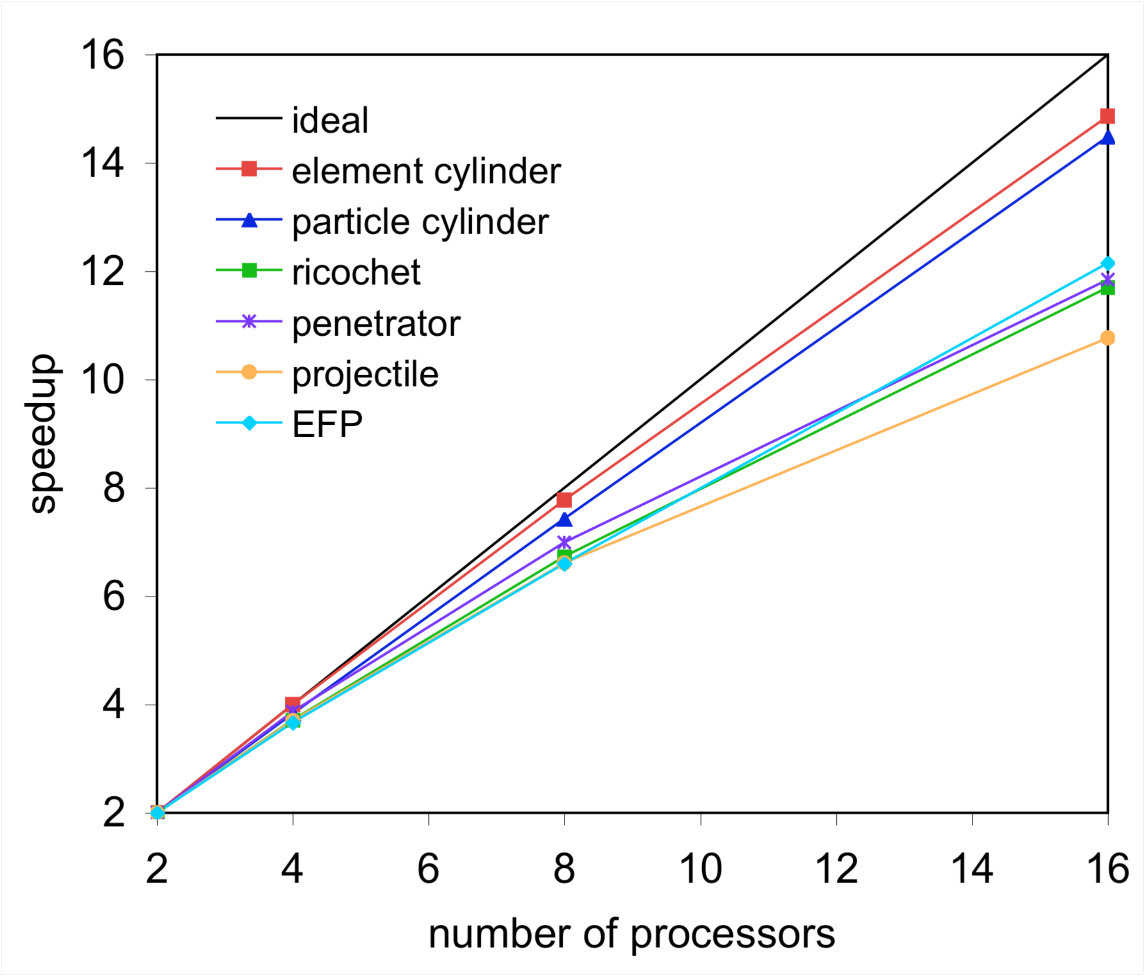
- **Performance**
  - **No function calls for communication**
    - No function call overhead
    - Compilers can optimize inter-processor communication
    - Non-native CAF compilers don’t have these advantages
- **Productivity**
  - **CAF Fortran syntax often more readable than complex MPI calling sequence**

EPIC Overview

- **Elastic-Plastic Impact Computations**
- A finite element code used to simulate projectile-target interaction
- Complex phenomena
- Computationally intensive
- Large legacy code initially developed for serial execution



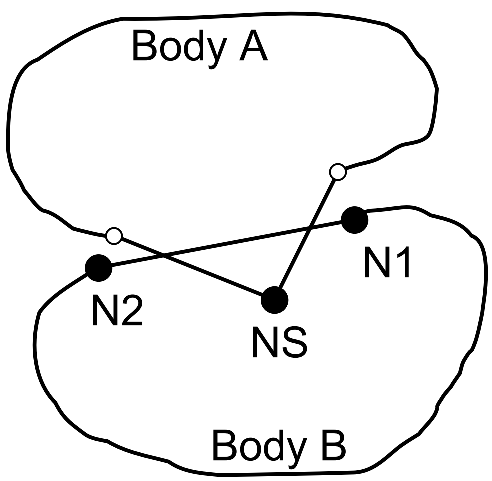
MPI Scaling of EPIC Cases



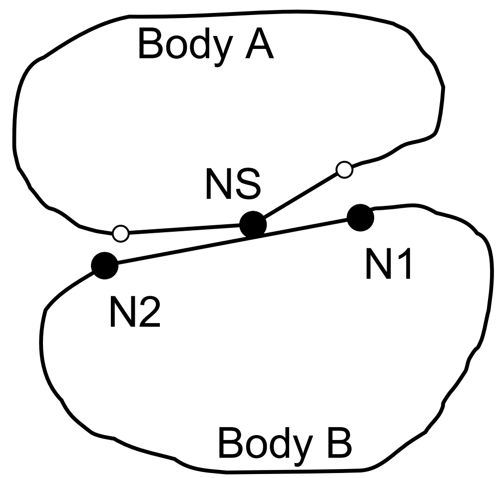
Contact Algorithm Overview

- Simulating contact of multiple bodies is a critical feature of EPIC
- When bodies make contact, nodes 'penetrate' surfaces
- The contact algorithm consists of iterative adjustment to eliminate penetration

Before Adjustment



After Adjustment



Contact Scalability Issues

- Contact between bodies is unpredictable
  - Good load balancing is tricky
  - Inter-processor communication is complex
- The contact algorithm is iterative
  - Inter-processor communication is frequent
  - Latency limits scaling

CAF Parallel Performance Optimizations

- Low latency communication
  - Critical when messages are small
- Fine-grain communication hiding
  - Work on incoming data as it arrives, rather than waiting
  - A form of *pipelining*
  - Uniquely valuable when no independent work is available to hide communication time

Example 1: Low Latency

- **CAF code 8 times faster than MPI**
  - **Latency advantage important for small messages**

Original Code:

```
CALL  MPI_ALLGATHER(NUMALTERED,1,
      MPI_INTEGER,ITMP,NUM,MPI_INTEGER,
       MPI_COMM_WORLD,IER)
```

CAF Code:

```
DO I=1,NPES
    ITMP(I)=NUMALTERED(1)[I]
ENDDO
```

Example #2: Fine-Grain Communication Hiding

Original Code:

- The computations in the loop cannot begin until the 4 MPI_ALLREDUCE calls finish
- Unnecessary computation & communication for many elements of PX, PY, and PZ whose values are 0.0

```
TEMP(1:SLDTOT)=PX(1:SLDTOT)
CALL MPI_ALLREDUCE(TEMP, PX, SLDTOT,   &
                   MPI_DOUBLE_PRECISION,   &
        MPI_SUM, MPI_COMM_WORLD, IER)
TEMP(1:SLDTOT)=PY(1:SLDTOT)
CALL MPI_ALLREDUCE(TEMP, PY, SLDTOT,    &
                   MPI_DOUBLE_PRECISION,   &
         MPI_SUM, MPI_COMM_WORLD, IER)
TEMP(1:SLDTOT)=PZ(1:SLDTOT)
CALL MPI_ALLREDUCE(TEMP, PZ, SLDTOT,     &
                   MPI_DOUBLE_PRECISION,    &
              MPI_SUM, MPI_COMM_WORLD, IER)
LTEMP(1:SLDTOT)=UPDATE(1:SLDTOT)
CALL MPI_ALLREDUCE(LTEMP,UPDATE,SLDTOT, &
                         MPI_LOGICAL,MPI_LOR, &
                        MPI_COMM_WORLD,IER)
DO M=1,SLDTOT
   IF (UPDATE(M)) THEN
      CALL NFIX(IXYZ(M),IRIG,IXX,IYY,IZZ)
      X(M) = X(M) + PX(M)*(1-IXX)
      Y(M) = Y(M) + PY(M)*(1-IYY)
      Z(M) = Z(M) + PZ(M)*(1-IZZ)
   ENDIF
ENDDO
```

Example #2: Fine-Grain Communication Hiding

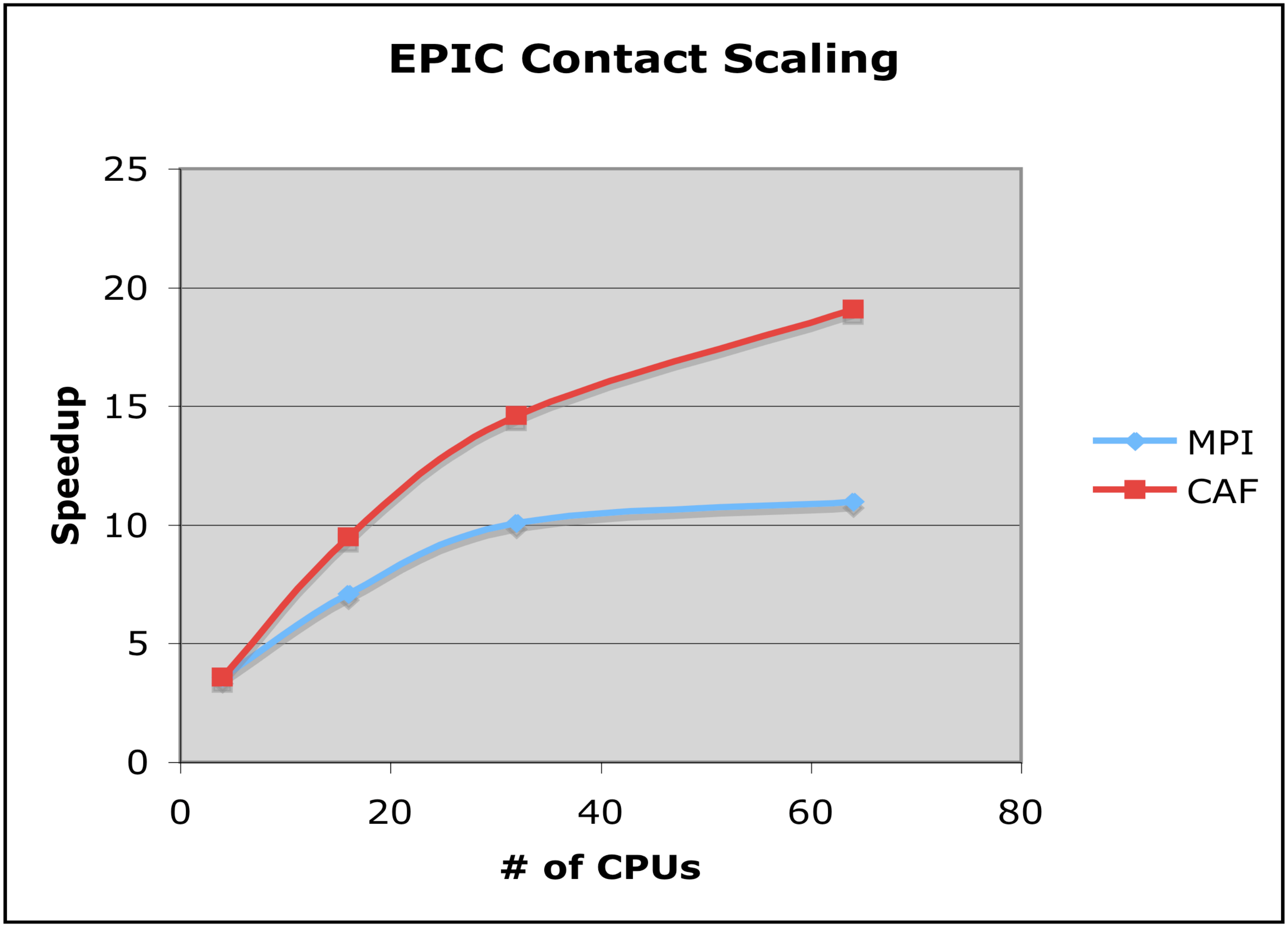
CAF Code:

```
ICOUNT=0
DO I=1,SLDTOT
  IF (UPDATE(I)) THEN
    ICOUNT=ICOUNT+1
    ICTEMP(ICOUNT)=I
    PXTEMP(ICOUNT)=PX(I)
    PYTEMP(ICOUNT)=PY(I)
    PZTEMP(ICOUNT)=PZ(I)
  ENDIF
ENDDO
CALL SYNC_IMAGES()

DO ITER=1,NPES
  ISRC=MYPN-ITER+1
  IF (ISRC.LE.0) ISRC=ISRC+NPES
    DO M=1,ICOUNT[ISRC]
      GLOB=ICTEMP(M)[ISRC]
      CALL NFIX(IXYZ(GLOB),IRIG,IXX,IYY,IZZ)
      X(GLOB)=X(GLOB)+PXTEMP(M)[ISRC]*(1-IXX)
      Y(GLOB)=Y(GLOB)+PYTEMP(M)[ISRC]*(1-IYY)
      Z(GLOB)=Z(GLOB)+PZTEMP(M)[ISRC]*(1-IZZ)
    ENDDO
ENDDO
```

- Only non-zero values are communicated
- Virtually all communication is 'hidden' by concurrent computations
  - Vector loads directly from remote memory
- 5 times as fast as the original MPI code

Performance Results



Observations

- CAF significantly faster for latency-sensitive communication
- CAF allows fine-grain communication hiding not possible with MPI
- The implementation matters
  - Requires underlying support for pipelining remote memory operations
- CAF offers a natural way to take full advantage of high performance hardware
- Adding CAF to MPI is painless (on the X1E)
- If pipelining is important to 'hide' local memory operations (it is), it must be *really* important for hiding remote memory operations