Optimization of the Poisson Operator in Chombo

Razvan Carbunescu, Meriem Ben Salah
and
Andrew Gearhart

Research supported by Microsoft (Award #024263) and Intel (Award #024894) funding and by matching funding by U.C. Discovery (Award #DIG07-10227)

Administrivia: The emu is watching you

Outline

- Introduction
  - Why the Poisson operator?
  - What is Chombo?
- Theoretical Background
- Targeted Architectures
- Implementation
- Challenges

Outline

- Results
  - Serial Implementation
  - pthreads
  - OpenMP
  - GPU (GTX280)
- Future Work

Introduction: Why the Poisson Operator?

- The Poisson operator is a key component of the Poisson equation

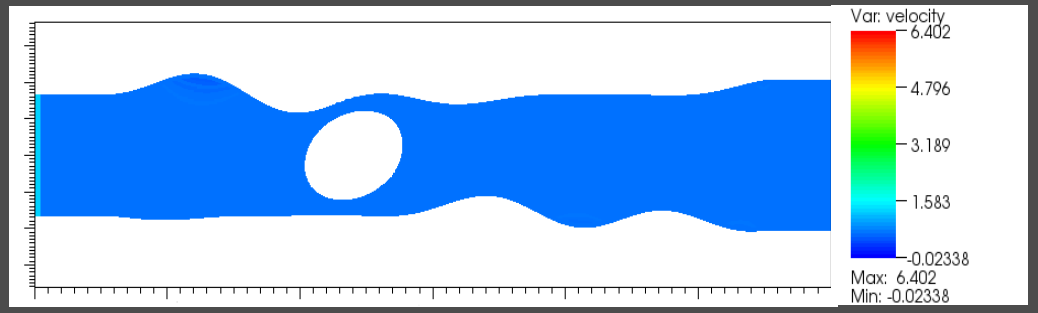


Figure: Flow Evolution startup after Poisson solve

- A Poisson solution is the first step toward solving incompressible Navier-Stokes equations for fluid flow

- Parlab Health Application

  - Modeling blood flow through cerebral arteries

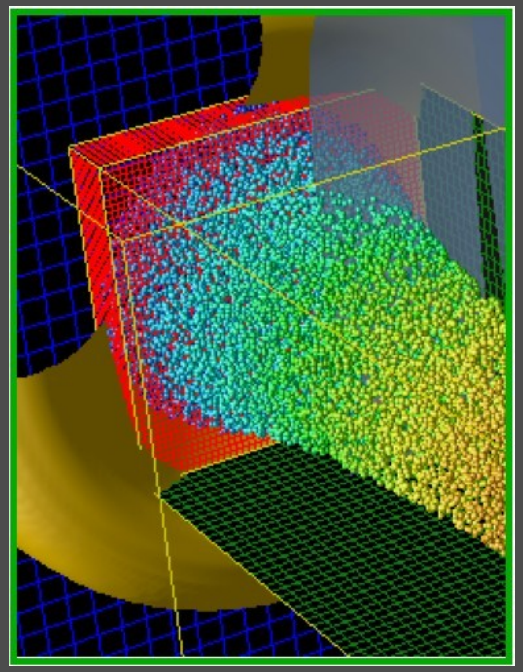


Figure: Particle-In-Cell simulation from LBL using Chombo

Introduction: Why the Poisson Operator?

- The Poisson operator is a key component of the Poisson equation

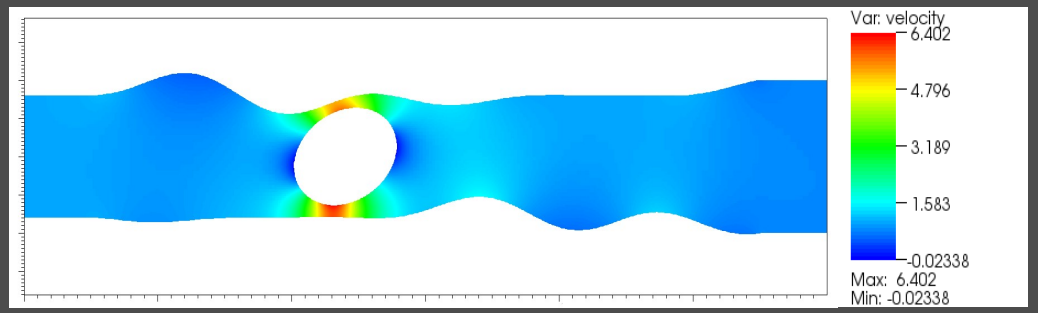


Figure: Flow Evolution startup after Poisson solve

- A Poisson solution is the first step toward solving incompressible Navier-Stokes equations for fluid flow

- Parlab Health Application

  - Modeling blood flow through cerebral arteries

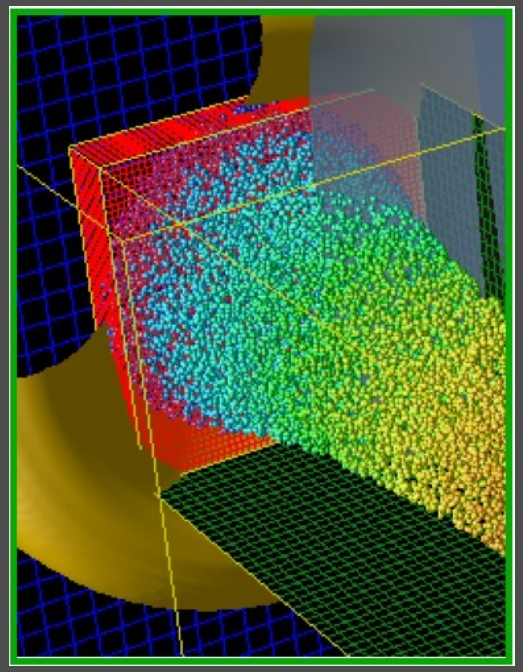


Figure: Particle-In-Cell simulation from LBL using Chombo

Introduction: What is Chombo?

- Developed and distributed by the Applied Numerical Algorithms Group of Lawrence Berkeley National Lab

- a framework to implement finite difference methods for the solution of PDEs on block structured, adaptively refined grids.

- Chombo provides elliptic and time-dependent modules, as well as support for standardized self-describing file formats.

- Chombo is architecture and operating system independent.

Introduction: What is Chombo?

- For parallel platforms, Chombo provides a distributed memory implementation using the Message Passing Interface (MPI) library

- This begs the question:

Introduction: What is Chombo?

- For parallel platforms, Chombo provides a distributed memory implementation using the Message Passing Interface (MPI) library

- This begs the question:

  Is a distributed memory implementation always the most efficient?

Introduction: What is Chombo?

- For parallel platforms, Chombo provides a distributed memory implementation using the Message Passing Interface (MPI) library

- This begs the question:

  Is a distributed memory implementation always the most efficient?

- One of the major components of Chombo is a collection of Multigrid (MG) solvers for discretized elliptic problems, including Poisson's Equation

- This portion of the Chombo suite has been modified to explore the above question

Introduction: Strategy and Goals

- Determine whether we can improve Chombo performance through the use of locality and faster access time to on-chip cores
  - Via different models of parallel execution and specialized hardware (ie. the GPU)

- Identify critical “crossover” points where one algorithm becomes more efficient (if they exist)

- Hopefully foster the creation of heterogeneous systems that automatically adapt execution to utilize distributed/shared memory or the GPU to enhance performance

Theoretical Background

- The Poisson operator, aka the Laplacian, is a second order elliptic differential operator and defined in an n-dimensional Cartesian space by:

$$\text{Given a function } \Phi \text{ the Laplacian operator is given by } \triangle \Phi = \sum_{i=1}^{n} \frac{\partial^2 \Phi}{\partial x_i^2}$$

- The Poisson operator appears in the definition of the Helmholtz differential equation:

$$\Phi + \beta \triangle \Phi = f$$

  - The Helmholtz differential equation reduces to the Poisson equation:

$$\text{if } \alpha = 0, \text{then } \beta \triangle \Phi = f$$

Theoretical Background

- The definition of appropriate boundary conditions, Dirichlet or Neumann, allows for the solution of the Poisson problem

- A numerical solution requires the discretization of the continuous Poisson's equation, e.g. by the standard centered-difference approximation, as well as a discrete handling of the boundary conditions

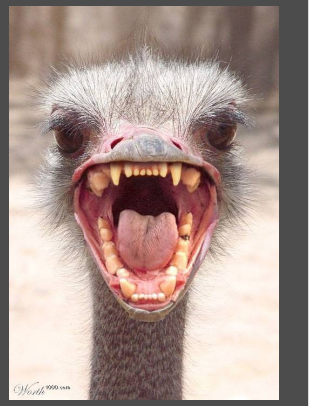
- The discrete Poisson operator, the focus of this project, is given by the following stencil:

$$(\triangle^h \Phi_i) \approx \frac{1}{h^2} \sum_{d=0}^{D-1} (\Phi_{i+e^d} + \Phi_{i-e^d} - 2\Phi_i), \text{where } h \text{ is the grid size,}$$

i is the index of the cell-centered data of interest,

D is the domain dimension, and e^d ias the grid director

Targeted Architectures



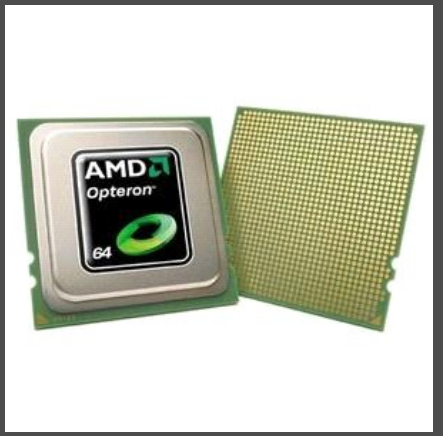
Existing Implementations:

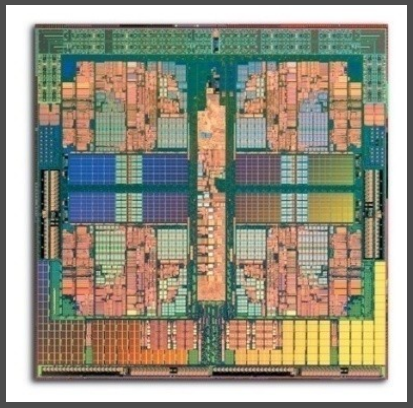
- Chombo's implementation is currently tuned for distributed memory with the domain being decomposed into small bins (32^3 elements for 3D) and individual bin computations are allocated for execution via serial f77 codes

- Because of the small size of bins there is a small amount computational intensity to use a threaded shared memory implementation or to hide the cost of GPU memory transfers

Targeted Architectures

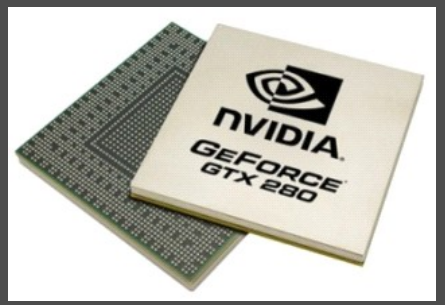
- **Our interest:**
  - Could Chombo be optimized for different models of parallel computation if the bin sizes were increased?
  - We would like to implement shared memory computation models utilizing:
    - OpenMP
    - Pthreads
      - lightweight threads may perform well with small bins

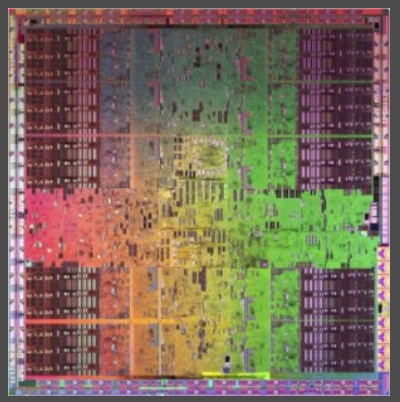




Targeted Architectures

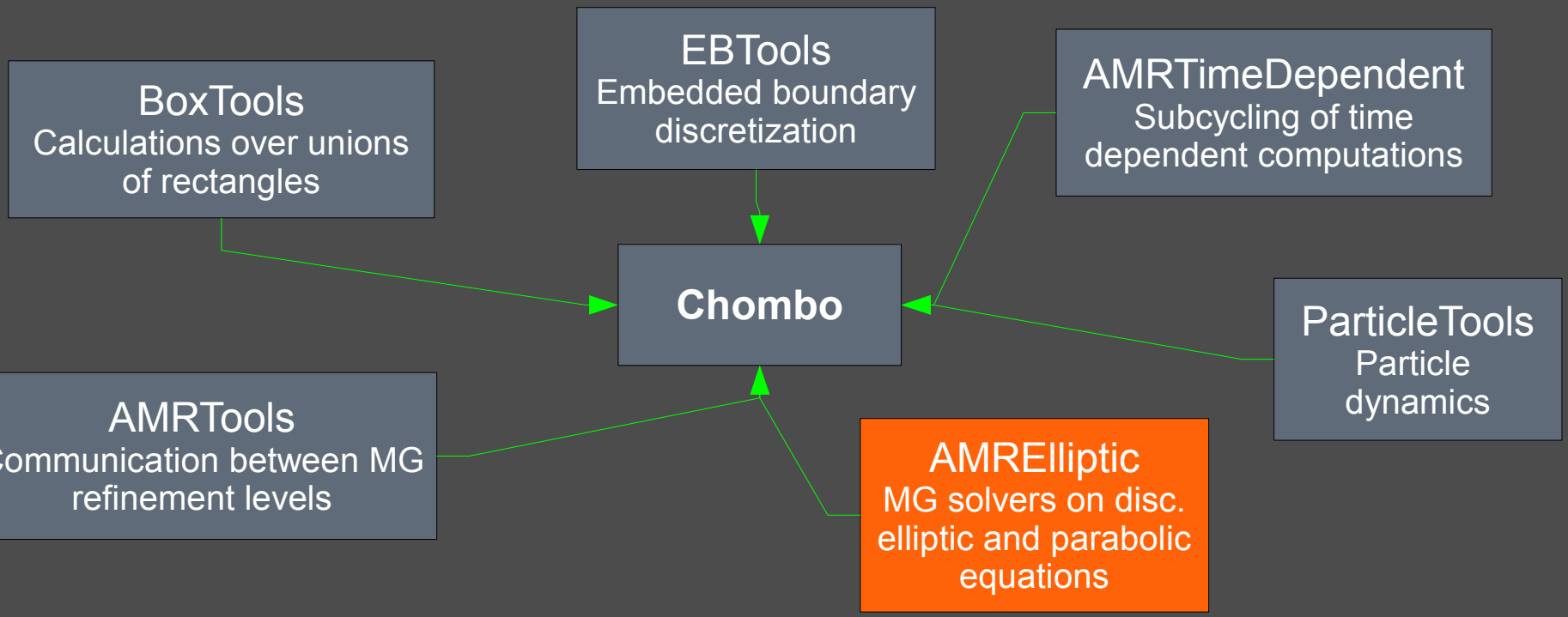
- **Our interest:**
  - Another interesting opportunity for speedup is running the operator on the GPU
    - benefits must outweigh the data transfer cost
  - GPU execution offers a highly-parallel execution environment with proven performance for stencil codes
    - uncoalesced memory accesses can be problematic





Implementation

- Chombo is implemented in C++ utilizing a complex set of templates and classes
- Bottom-level computation is performed in Fortran 77 via the Fortran/C interface
- Key components of the software package are grouped accordingly:



Implementation

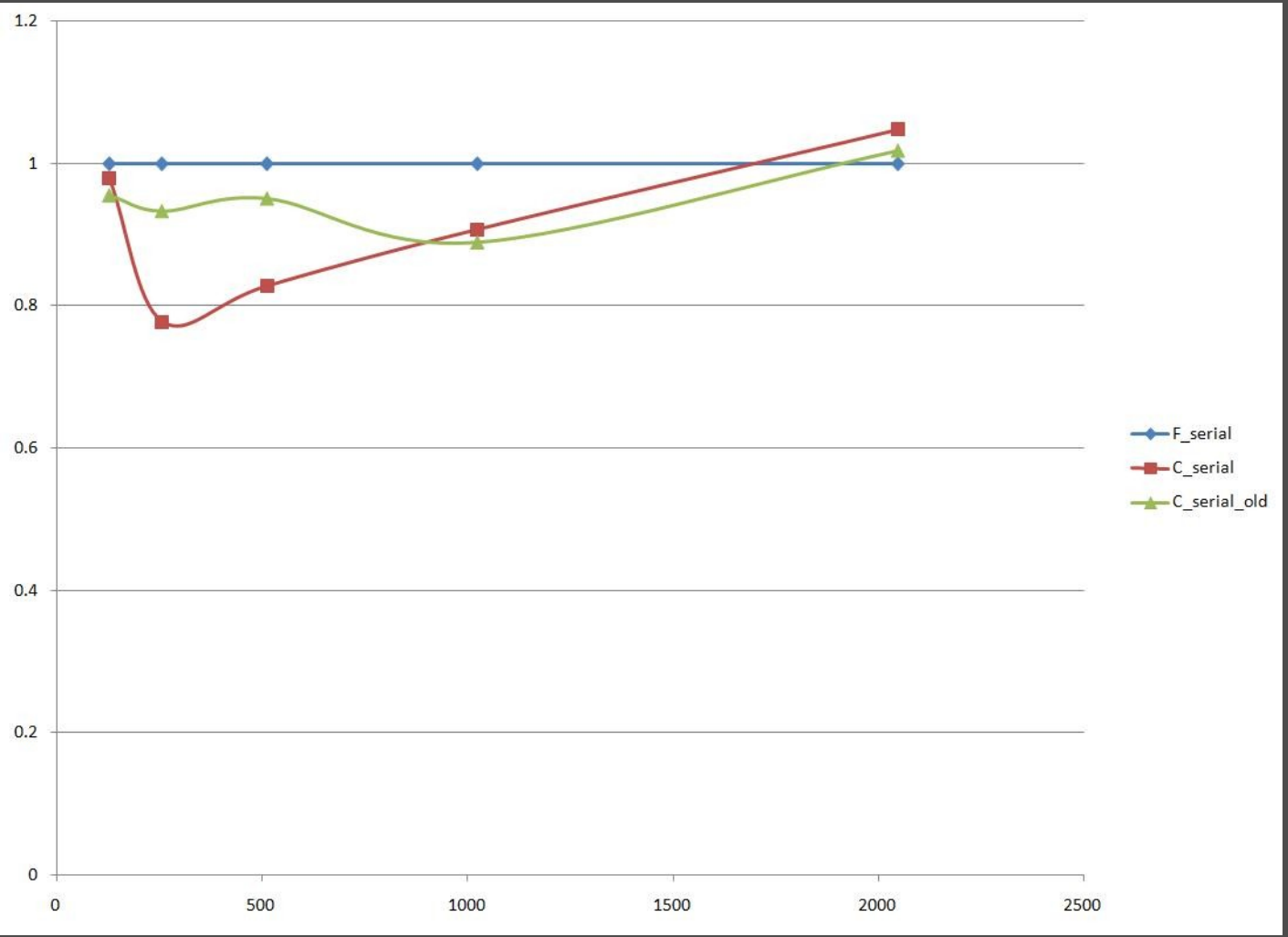
- Low-level C functions replace Fortran 77 kernels
  - Performance implications?
- Bad coding style:
  - “ghetto hack” or “feature development”?
  - abstract class hierarchy was bypassed to access data arrays directly
  - arrays are stored in Fortran column-major order, and then modified within C functions
    - problems with memory indexing
  - only have access to already-decomposed computational regions
    - limited to 2048 elements cubed

Results: Serial Implementation

- **Methods**:
  - used GNU compiler suite: g++ and gfortran 4.2.0
  - Implemented Poisson operator with a C function instead of Fortran 77
  - A version of the C code utilizes the “__restrict__” type qualifier and “-fstrict-aliasing” to declare parameters as non-aliased

Results: Serial Implementations

Problem Size vs. Serial code runtime (applyOp)

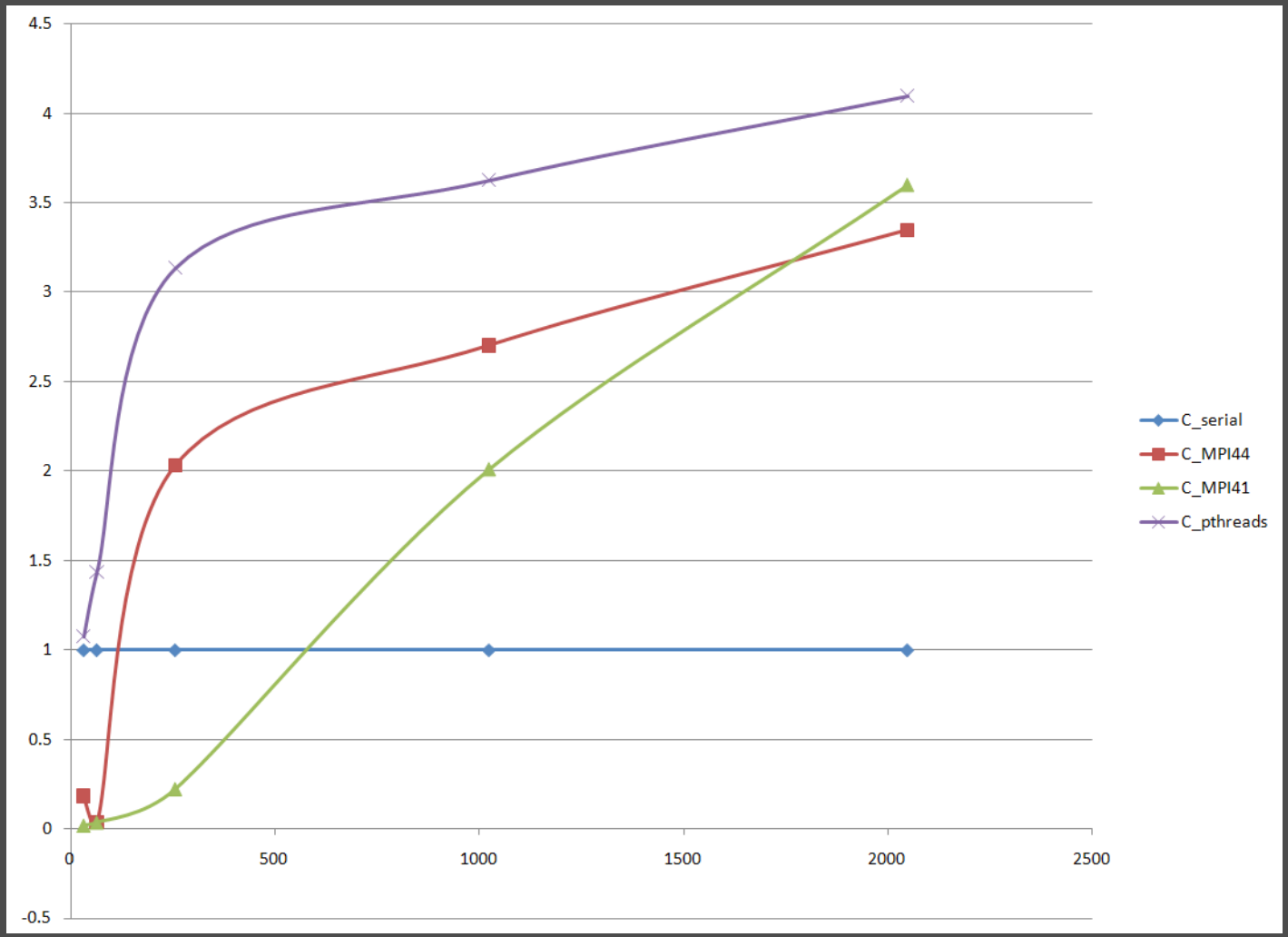


Results: Pthreads

- **Methods**:
  - Utilized the standard pthread library to implement a parallel code that runs on-chip without the overhead of MPI
  - Threaded code was run on NERSC's Cray XT4 (“Franklin”)
    - Quad-core, 64-bit AMD Opteron nodes
  - Codes were run with 4 threads to explore node-local performance

Results: Pthreads

Problem Size vs. Speedup over C serial (applyOp)



Results: OpenMP and GPU

- **Methods**:

  - OpenMP
    - The OpenMP implementation is implemented via code directives that indicate parallel sections of code

    - This promises access to an abstract and powerful way to parallelize codes

  - GPU
    - Due to convergence problems in single-precision, the double-precision nVidia GTX280 was the focus of experimentation

    - Stencil code was written in using NVidia's Cuda extensions to the C programming language

Results: OpenMP and GPU

- Data collection pending:

  - Compilation errors for OpenMP code

  - Indexing for the Cuda version of the solve is currently in error

  - Currently, the Cuda stencil is a very naïve implementation and does not optimize using blocking for registers and shared memory

Future Work

- more complicated memory optimizations
    - circular queues
    - time skewing

- better GPU memory coalescing
    - blocking
    - padding

- using the GPU's other memory
    - constant
    - texture

- interpolation via texture cache hardware

Fin.

Thanks to all our colleagues at LBL and at UC Berkeley for their gracious help in the development of this project.

Administrivia: We got the emu