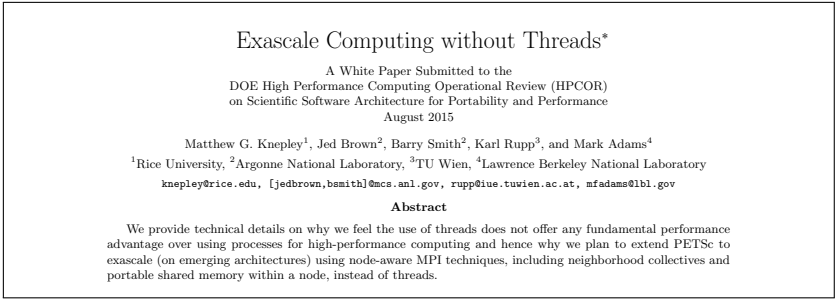
Exascale Computing Without Templates

Karl Rupp, Richard Mills, Barry Smith, Matthew Knepley, Jed Brown

Argonne National Laboratory

DOE COE Performance Portability Meeting, Denver
August 22-24, 2017

Providing Context



Exascale Computing without Threads*

A White Paper Submitted to the
DOE High Performance Computing Operational Review (HPCOR)
on Scientific Software Architecture for Portability and Performance
August 2015

Matthew G. Knepley[1], Jed Brown[2], Barry Smith[2], Karl Rupp[3], and Mark Adams[4]
[1]Rice University, [2]Argonne National Laboratory, [3]TU Wien, [4]Lawrence Berkeley National Laboratory
knepley@rice.edu, [jedbrown,bsmith]@mcs.anl.gov, rupp@iue.tuwien.ac.at, mfadams@lbl.gov

Abstract

We provide technical details on why we feel the use of threads does not offer any fundamental performance advantage over using processes for high-performance computing and hence why we plan to extend PETSc to exascale (on emerging architectures) using node-aware MPI techniques, including neighborhood collectives and portable shared memory within a node, instead of threads.

https://www.orau.gov/hpcor2015/whitepapers/Exascale_Computing_without_Threads-Barry_Smith.pdf

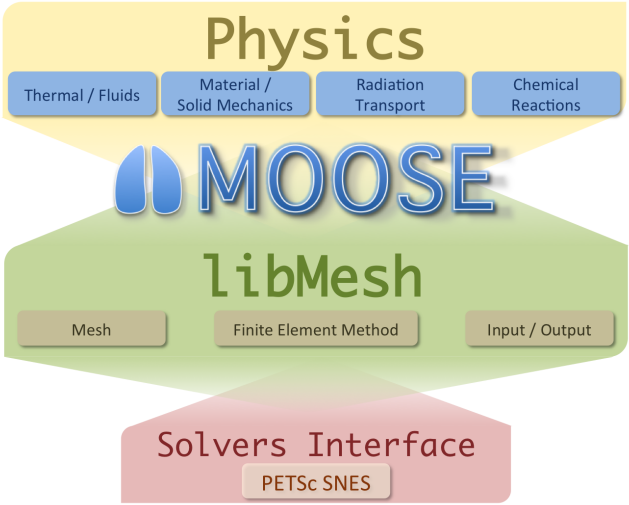
PETSc Developers Care About Recent Developments

After careful evaluation: Favor MPI 3.0 (and later) over threads

Find the best long-term solutions for our users

Consider best solutions for large-scale applications, not just toy-apps

Providing Context



http://mooseframework.org/static/media/wiki/images/229/b61cdbc1e8be71dae37adc31a688d209/moose-arch.png

Providing Context

Our Attempts in C++ Library Development

Sieve: Several years of C++ mesh management attempts in PETSc

ViennaGrid 2.x: Heavily templated C++ mesh management library

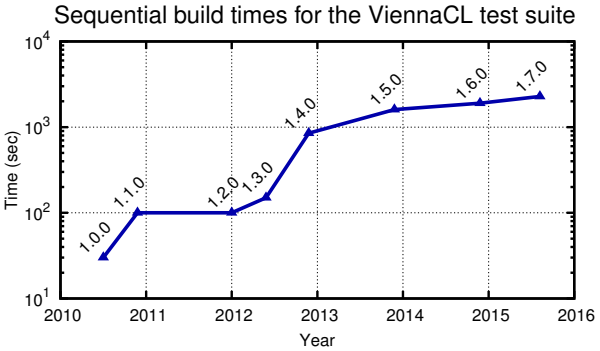
ViennaCL: Dense and sparse linear algebra and solvers for multi- and many-core architectures

Aftermath

Sieve: Replaced by DMPlex (written in C)

ViennaGrid: Version 3.0 provides C-ABI

ViennaCL: Rewrite in C likely



Disadvantages of C++ Templates

Static Dispatch

Architecture-specific information only available at run time

“Change code and recompile” not acceptable advice

Dealing with Compilation Errors

Type names pollute compiler output

Replicated across interfaces

CRTP may result in type length explosion

Default arguments become visible

https://xkcd.com/303/

Type	Length
`std::vector<int>`	38
`std::vector<std::vector<int> >`	109
`std::vector<std::vector<std::vector<int> > >`	251
`std::vector<std::vector<std::vector<std::vector<int> > > >`	539

Disadvantages of C++ Templates

https://tgceec.tumblr.com/

Disadvantages of C++ Templates

Scope Limitations

Template metaprogramming lacks state

Optimizations across multiple code lines difficult or impossible

Example

Consider vector updates in pipelined CG method:

$$x_i \leftarrow x_{i-1} + \alpha p_{i-1}$$
$$r_i \leftarrow r_{i-1} - \alpha y_i$$
$$p_i \leftarrow r_i + \beta p_{i-1}$$

Reuse of p_{i-1} and r_{i-1} easy with for-loops, but hard with expression templates

Disadvantages of C++ Templates

Complicates Debugging

- Stack traces get longer names and deeper
- Setting good breakpoints may become harder

Lack of a Stable ABI

- Object files from different compilers generally incompatible
- Name mangling makes use outside C++ land almost impossible

High Entry Bar

- Number of potential contributors inversely proportional to code sophistication
- Domain scientists have limited resources for C++ templates

A Path Forward

Manage Complexity

Good interface design

Refactor code when needed

Hand-optimize small kernels only (cf. BLIS methodology)

Development Implications

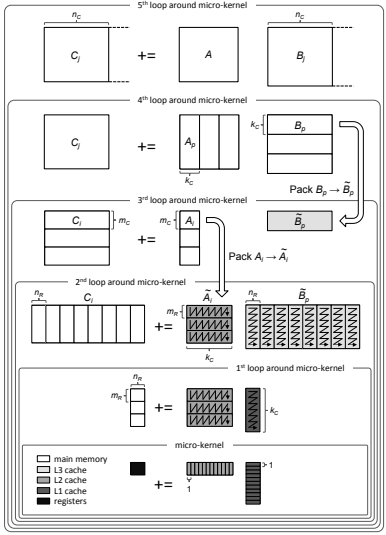
Adopt professional software development practices

Develop, maintain, and evolve different datastructures ...

... and code paths

Use clear and easy-to-understand datastructures

Fallacy: “Writing” an application only once in its final form



[F. Van Zee, T. Smith, ACM TOMS 2017]

A Path Forward

Spending Development Resources

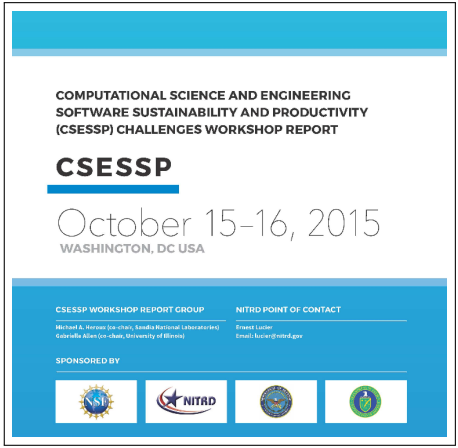
- Reuse existing libraries — reinventing the wheel is not productive!
- Focus on domain- and application-specific aspects
- Obtain expertise and resources for continuous code evolution

Required Incentives

- Reward contributions to existing projects
- Pair research funding with software development funding
- Establish software development career tracks

A Path Forward

Is Performance Portability Just a Software Productivity Aspect?



https://www.nitrd.gov/PUBS/CSESSPWorkshopReport.pdf

Summary

Long-Term Problems of Heavy C++ Templates Use

- Template metaprogramming is a leaky abstraction
- Excessive type names slow down all stages of Compile-Run-Debug-cycle
- Templates operate at compile time - architecture ultimately known at run time

A Path Forward

- Adopt professional software development practices
- Be prepared to develop different datastructures and code paths
- Write clear, readable code using simple datastructures
- Evolve and refactor datastructures, kernels, and interfaces over time
- *(cf. software productivity discussions)*