Porting Machine Learning and Modeling from a Laptop to a Supercomputer: Numerical Libraries

Matthew Knepley

Portable

Extensible

Toolkit for

Scientific

computing

https://petsc.org

Earth Science with PETSc

- PyLith (CIG)
- Underworld (Monash)
- Salvus (ETHZ)
- TerraFERMA (Columbia)
- PFLOTRAN (DOE)
- STOMP (DOE)
- pTatin3d (UCSD)
- Rhea (NYU)
- Waiwera (U Auckland)

Sparse, Parallel Linear Algebra

- Vec/Mat bound to a compute resource at runtime
  "Toward Performance-Portable PETSc for GPU-based Exascale Systems"
  arXiv:2011.00715

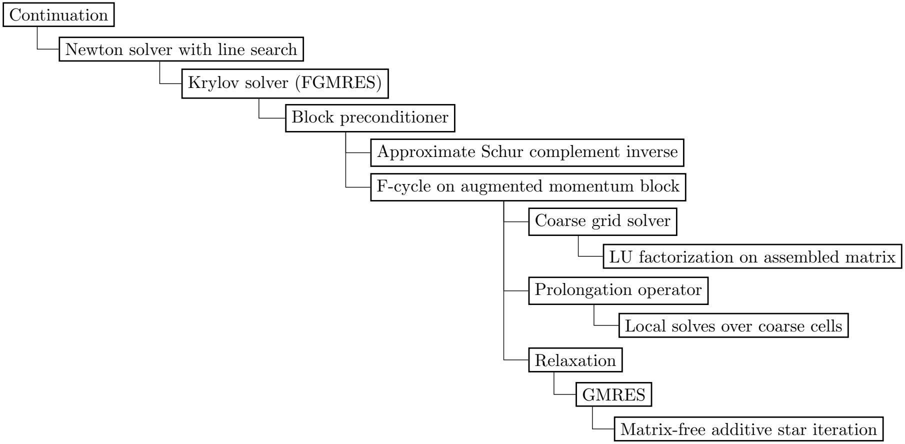
- Communication happens directly between GPUs
  "The PetscSF Scalable Communication Layer"
  arXiv:2102.13018

Implicitness

- Allow accuracy limits to supercede stability
  - CFL limits
  - Geometric limits
- Scale separation
  - Parabolization
  - Localization
- Inverse problems
  - Bayesian inference
  - Parameter estimation

Composable Solvers

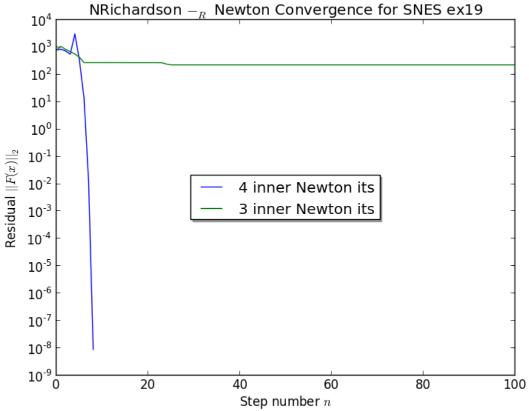
Linear


Continuation
Newton solver with line search
Krylov solver (FGMRES)
Block preconditioner
Approximate Schur complement inverse
F-cycle on augmented momentum block
Coarse grid solver
LU factorization on assembled matrix
Prolongation operator
Local solves over coarse cells
Relaxation
GMRES
Matrix-free additive star iteration

Farrell, Mitchell, and Wechsung (2018), arXiv:1810.03315

Preconditioning NRichardson with Newton

```
./ex19 -lidvelocity 100 -grashof 1.3373e2
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type nrichardson -snes_max_it 200
  -npc_snes_type newtonls -npc_snes_max_it 3 -npc_pc_type lu
```



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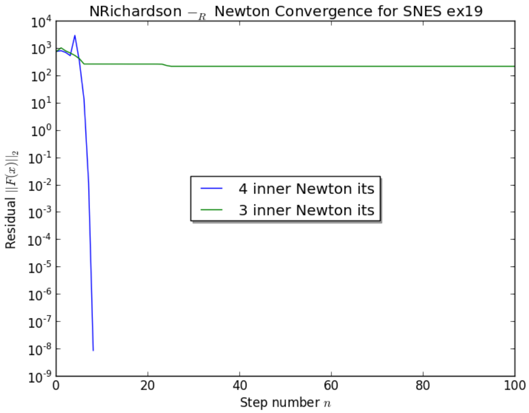
  -npc_snes_type newtonls -npc_snes_max_it 4 -npc_pc_type lu
```



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  -snes_type newtonls -snes_max_it 1000 -pc_type lu
  -npc_snes_type nrichardson -npc_snes_max_it 1
```

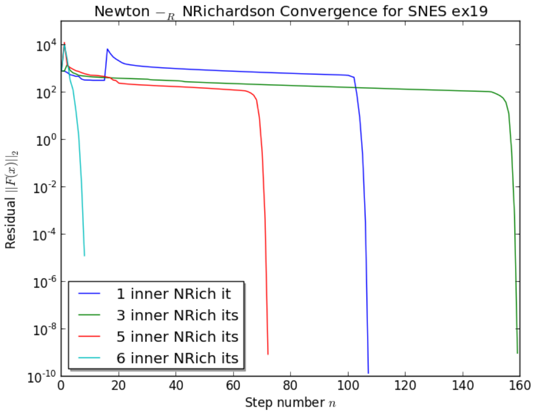

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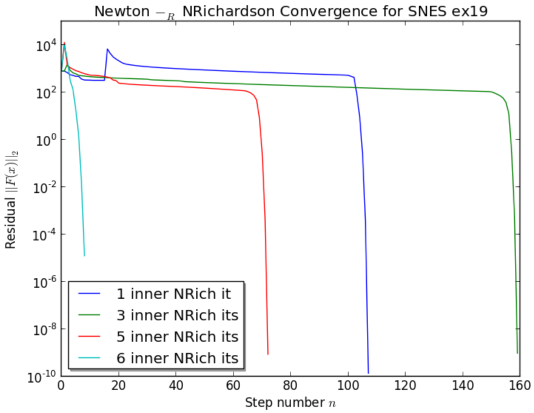

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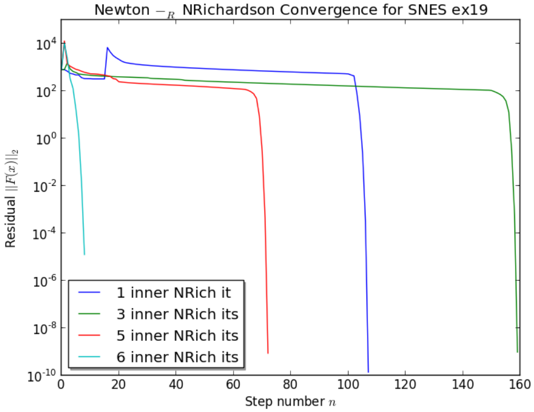
  -snes_type newtonls -snes_max_it 1000 -pc_type lu
  -npc_snes_type nrichardson -npc_snes_max_it 5
```



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```
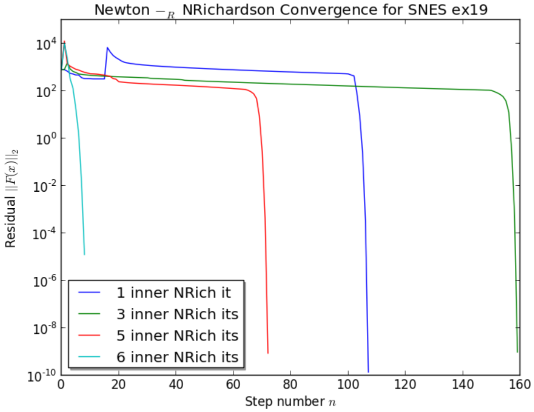
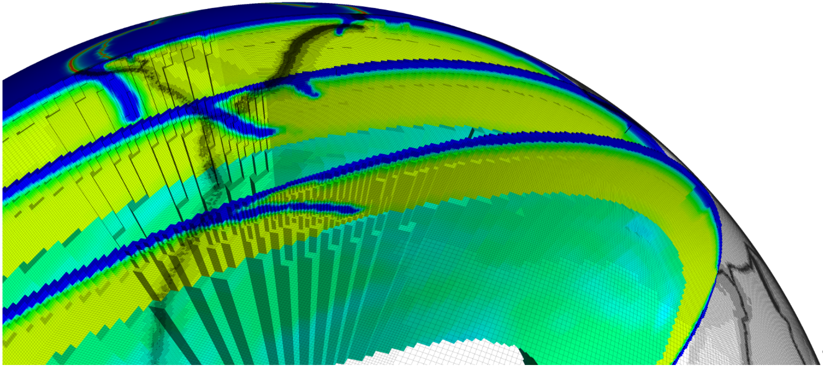



Adaptive Mesh Refinement

- DM interface with p4est package from Burstedde and Isaac
- PETSc solvers can be used seamlessly
- 2015 Gordon Bell Winner for Mantle Convection Simulation

[a]

[a]Isaac

Adaptive Mesh Refinement

- DM interface with p4est package from Burstedde and Isaac
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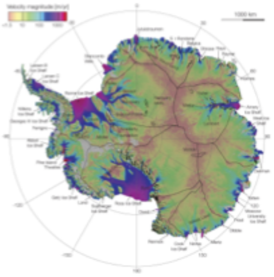
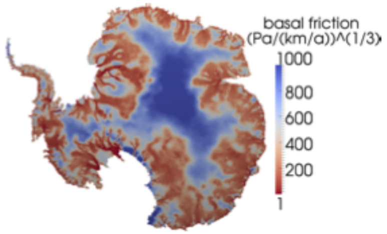
- Inversion for basal traction on the full Antarctic ice sheet



Observed surface flow velocity (Rignot et al., 2011)



Antarctic ice sheet inversion for the basal friction parameter field using InSAR surface velocity measurements [a]

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Adaptive Mesh Refinement

- DM interface with ParMmg package from Froehly and Cirrottola
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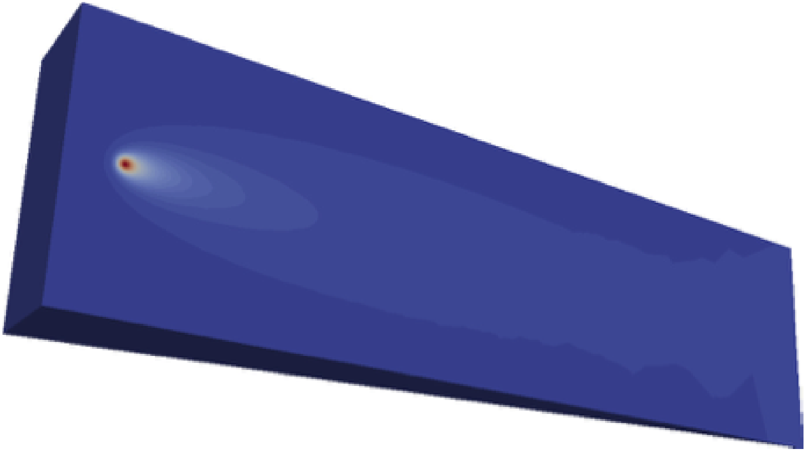
- Wallwork, Barral, Ham, Piggot (2021) eartharXiv:4205

[a]

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[a]Wallwork

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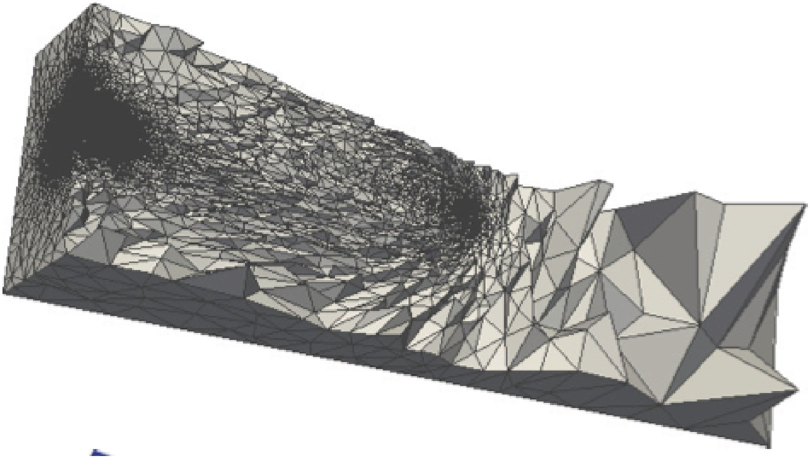
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Differentiability

- Low-level AD
  - PyTorch, Tensorflow
  - Enzyme
    “Performance-Portable Solid Mechanics via Matrix-Free *p*-Multigrid”
    arXiv:2204.01722
- High-level AD
  - pyadjoint (Firedrake, FEniCS)
    github:dolfin-adjoint/pyadjoint
  - libadjoint
    bitbucket:dolfin-adjoint/libadjoint

Why Libraries?

Libraries Hide
Hardware Details

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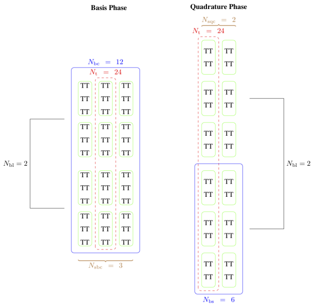

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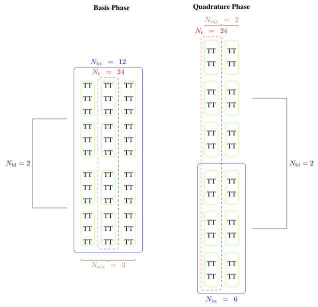

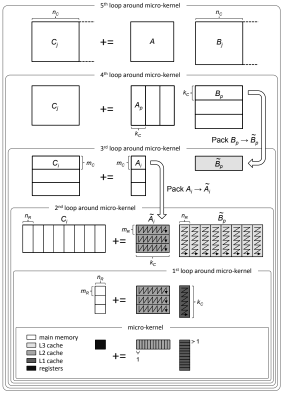

5th loop around micro-kernel
4th loop around micro-kernel
3rd loop around micro-kernel
2nd loop around micro-kernel
1st loop around micro-kernel
micro-kernel
n_C
C_j
+=
A
B_j
A_p
B_p
k_C
Pack $B_p \rightarrow \tilde{B}_p$
C_i
m_C
A_i
$\tilde{B}_p$
Pack $A_i \rightarrow \tilde{A}_i$
n_R
m_R
$\tilde{A}_i$
main memory
L3 cache
L2 cache
L1 cache
registers
1

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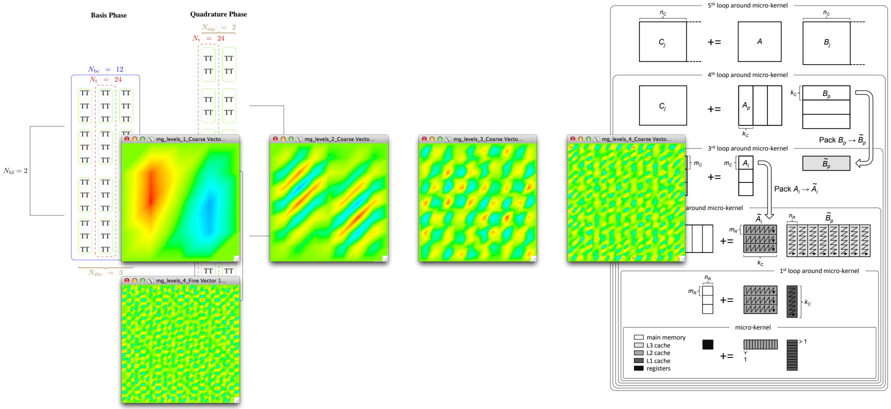

Basis Phase
Quadrature Phase
$N_{sqc} = 2$
$N_t = 24$
$N_{bc} = 12$
$N_t = 24$
$N_{bl} = 2$
$N_{sbc} = 3$
TT
mg_levels_1_Coarse Vecto...
mg_levels_2_Coarse Vecto...
mg_levels_3_Coarse Vecto...
mg_levels_4_Coarse Vecto...
mg_levels_4_Fine Vector 1...
5th loop around micro-kernel
n_C
C_j
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m_C
A_i
$\tilde{B}_p$
Pack $A_i \rightarrow \tilde{A}_i$
around micro-kernel
$\tilde{A}_i$
n_R
m_R
1st loop around micro-kernel
micro-kernel
main memory
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Why Libraries?

Libraries Accumulate
Best Practices

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Classical Gram-Schmidt orthogonalization with selective reorthogonalization

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Eigen-estimation for AMG with Krylov bootstrap

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Improvement without code changes

Libraries Simplfy
Determining Provenance

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Rather than making build-time choices,

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Rather than making build-time choices,
that must be plumbed through all levels
with another layer of workflow scripts
and brittle top-level interfaces,

Libraries Simplfy Determining Provenance

we use packages without modification,

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we use packages without modification, compiled in a standard way

Libraries Simplfy Determining Provenance

we use packages without modification,
compiled in a standard way
and controlled entirely via runtime options.

Why PETSc?

- Dependability & Maintainability
- Portability & Robustness
- Performance & Scalability
- Optimality & Robustness

- Flexibility & Extensibility

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- Dependability & Maintainability
  - Nearly 30 years of continuous development
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- Portability & Robustness
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  - Many Gordon Bell Winners
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    - State-of-the-Art Linear and Nonlinear Solvers, Eigensolvers, Optimization Solvers, Timesteppers
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  - More than 8000 citations and hundreds of application packages
  - Aerodynamics, Arterial Flow, Corrosion, Combustion, Data Mining, Earthquake Mechanics, . . .