PETSc

Portable, Extensible Toolkit for Scientific Computation

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Before we start...

Goal of this Workshop

You are here to learn new things about HPC

Ask Questions

- Tell me if you do not understand
- Ask for further details
- Don't be shy

Table of Contents

Debugging and Profiling

PETSc Debugging

By default, a debug build is provided

Launch the debugger

```
-start_in_debugger [gdb,dbx,noxterm]
-on_error_attach_debugger [gdb,dbx,noxterm]
```

Attach the debugger only to some parallel processes

```
-debugger_nodes 0,1
```

Set the display (often necessary on a cluster)

```
-display :0
```

Debugging Tips

- Put a breakpoint in `PetscError()` to catch errors as they occur
- PETSc tracks memory overwrites at both ends of arrays
  - The `CHKMEMQ` macro causes a check of all allocated memory
  - Track memory overwrites by bracketing them with `CHKMEMQ`
- PETSc checks for leaked memory
  - Use `PetscMalloc()` and `PetscFree()` for all allocation
  - Print unfreed memory on `PetscFinalize()` with `-malloc_dump`
- Simply the best tool today is Valgrind
  - It checks memory access, cache performance, memory usage, etc.
  - http://www.valgrind.org
  - Pass `-malloc 0` to PETSc when running under Valgrind
  - Might need `--trace-children=yes` when running under MPI
  - `--track-origins=yes` handy for uninitialized memory

Profiling

- Use `-log_summary` for a performance profile
  - Event timing
  - Event flops
  - Memory usage
  - MPI messages
- Call `PetscLogStagePush()` and `PetscLogStagePop()`
  - User can add new stages
- Call `PetscLogEventBegin()` and `PetscLogEventEnd()`
  - User can add new events
- Call `PetscLogFlops()` to include your flops

PETSc Profiling

Reading -log_view

```
                        Max        Max/Min        Avg      Total
Time (sec):           1.548e+02    1.00122   1.547e+02
Objects:              1.028e+03    1.00000   1.028e+03
Flops:                1.519e+10    1.01953   1.505e+10  1.204e+11
Flops/sec:            9.814e+07    1.01829   9.727e+07  7.782e+08
MPI Messages:         8.854e+03    1.00556   8.819e+03  7.055e+04
MPI Message Lengths:  1.936e+08    1.00950   2.185e+04  1.541e+09
MPI Reductions:       2.799e+03    1.00000
```

Also a summary per stage

Memory usage per stage (based on when it was allocated)

Time, messages, reductions, balance, flops per event per stage

Always send `-log_view` when asking
performance questions on mailing list

PETSc Profiling

Event	Count		Time (sec)		Flops					--- Global ---					--- Stage ---				
	Max	Ratio	Max	Ratio	Max	Ratio	Mess	Avg len	Reduct	%T	%F	%M	%L	%R	%T	%F	%M	%L	%R
--- Event Stage 1: Full solve																			
VecDot	43	1.0	4.8879e-02	8.3	1.77e+06	1.0	0.0e+00	0.0e+00	4.3e+01	0	0	0	0	0	0	0	0	0	1
VecMDot	1747	1.0	1.3021e+00	4.6	8.16e+07	1.0	0.0e+00	0.0e+00	1.7e+03	0	1	0	0	14	1	1	0	0	27
VecNorm	3972	1.0	1.5460e+00	2.5	8.48e+07	1.0	0.0e+00	0.0e+00	4.0e+03	0	1	0	0	31	1	1	0	0	61
VecScale	3261	1.0	1.6703e-01	1.0	3.38e+07	1.0	0.0e+00	0.0e+00	0.0e+00	0	0	0	0	0	0	0	0	0	0
VecScatterBegin	4503	1.0	4.0440e-01	1.0	0.00e+00	0.0	6.1e+07	2.0e+03	0.0e+00	0	0	50	26	0	0	0	96	53	0
VecScatterEnd	4503	1.0	2.8207e+00	6.4	0.00e+00	0.0	0.0e+00	0.0e+00	0.0e+00	0	0	0	0	0	0	0	0	0	0
MatMult	3001	1.0	3.2634e+01	1.1	3.68e+09	1.1	4.9e+07	2.3e+03	0.0e+00	11	22	40	24	0	22	44	78	49	0
MatMultAdd	604	1.0	6.0195e-01	1.0	5.66e+07	1.0	3.7e+06	1.3e+02	0.0e+00	0	0	3	0	0	0	1	6	0	0
MatMultTranspose	676	1.0	1.3220e+00	1.6	6.50e+07	1.0	4.2e+06	1.4e+02	0.0e+00	0	0	3	0	0	1	1	7	0	0
MatSolve	3020	1.0	2.5957e+01	1.0	3.25e+09	1.0	0.0e+00	0.0e+00	0.0e+00	9	21	0	0	0	18	41	0	0	0
MatCholFctrSym	3	1.0	2.8324e-04	1.0	0.00e+00	0.0	0.0e+00	0.0e+00	0.0e+00	0	0	0	0	0	0	0	0	0	0
MatCholFctrNum	69	1.0	5.7241e+00	1.0	6.75e+08	1.0	0.0e+00	0.0e+00	0.0e+00	2	4	0	0	0	4	9	0	0	0
MatAssemblyBegin	119	1.0	2.8250e+00	1.5	0.00e+00	0.0	2.1e+06	5.4e+04	3.1e+02	1	0	2	24	2	2	0	3	47	5
MatAssemblyEnd	119	1.0	1.9689e+00	1.4	0.00e+00	0.0	2.8e+05	1.3e+03	6.8e+01	1	0	0	0	1	1	0	0	0	1
SNESSolve	4	1.0	1.4302e+02	1.0	8.11e+09	1.0	6.3e+07	3.8e+03	6.3e+03	51	50	52	50	50	99	100	99	100	97
SNESLineSearch	43	1.0	1.5116e+01	1.0	1.05e+08	1.1	2.4e+06	3.6e+03	1.8e+02	5	1	2	2	1	10	1	4	4	3
SNESFunctionEval	55	1.0	1.4930e+01	1.0	0.00e+00	0.0	1.8e+06	3.3e+03	8.0e+00	5	0	1	1	0	10	0	3	3	0
SNESJacobianEval	43	1.0	3.7077e+01	1.0	7.77e+06	1.0	4.3e+06	2.6e+04	3.0e+02	13	0	4	24	2	26	0	7	48	5
KSPGMRESOrthog	1747	1.0	1.5737e+00	2.9	1.63e+08	1.0	0.0e+00	0.0e+00	1.7e+03	1	1	0	0	14	1	2	0	0	27
KSPSetup	224	1.0	2.1040e-02	1.0	0.00e+00	0.0	0.0e+00	0.0e+00	3.0e+01	0	0	0	0	0	0	0	0	0	0
KSPSolve	43	1.0	8.9988e+01	1.0	7.99e+09	1.0	5.6e+07	2.0e+03	5.8e+03	32	49	46	24	46	62	99	88	48	88
PCSetUp	112	1.0	1.7354e+01	1.0	6.75e+08	1.0	0.0e+00	0.0e+00	8.7e+01	6	4	0	0	1	12	9	0	0	1
PCSetUpOnBlocks	1208	1.0	5.8182e+00	1.0	6.75e+08	1.0	0.0e+00	0.0e+00	8.7e+01	2	4	0	0	1	4	9	0	0	1
PCApply	276	1.0	7.1497e+01	1.0	7.14e+09	1.0	5.2e+07	1.8e+03	5.1e+03	25	44	42	20	41	49	88	81	39	79

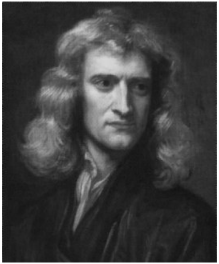
Communication Costs

- Reductions: usually part of Krylov method, latency limited
  - `VecDot`
  - `VecMDot`
  - `VecNorm`
  - `MatAssemblyBegin`
  - Change algorithm (e.g. IBCGS)
- Point-to-point (nearest neighbor), latency or bandwidth
  - `VecScatter`
  - `MatMult`
  - `PCApply`
  - `MatAssembly`
  - `SNESFunctionEval`
  - `SNESJacobianEval`
  - Compute subdomain boundary fluxes redundantly
  - Ghost exchange for all fields at once
  - Better partition

Nonlinear Solvers

Newton Iteration: Workhorse of SNES

Standard form of a nonlinear system



$$-\nabla \cdot \left(|\nabla u|^{\mathfrak{p}-2} \nabla u\right) - \lambda e^u = F(u) = 0$$

Iteration

$$\begin{aligned} \text{Solve:} \quad & J(u) w = -F(u) \\ \text{Update:} \quad & u^+ \leftarrow u + w \end{aligned}$$

- Quadratically convergent near a root: $|u^{n+1} - u^*| \in \mathcal{O}\left(|u^n - u^*|^2\right)$
- Picard is the same operation with a different $J(u)$

Jacobian Matrix for $\mathfrak{p}$-Bratu Equation

$$J(u) w \sim -\nabla \left[(\eta \mathbf{1} + \eta' \nabla u \otimes \nabla u) \nabla w \right] - \lambda e^u w$$

$$\eta' = \frac{\mathfrak{p}-2}{2} \eta / (\epsilon^2 + \gamma)$$

Scalable Nonlinear Equation Solvers

- Newton solvers: Line Search, Thrust Region
- Inexact Newton-methods: Newton-Krylov
- Matrix-Free Methods: With iterative linear solvers

How to get the Jacobian Matrix?

- Implement it by hand
- Let PETSc finite-difference it
- Use Automatic Differentiation software

Nonlinear solvers in PETSc SNES

LS, TR	Newton-type with line search and trust region
NRichardson	Nonlinear Richardson, usually preconditioned
VIRS, VISS	reduced space and semi-smooth methods for variational inequalities
QN	Quasi-Newton methods like BFGS
NGMRES	Nonlinear GMRES
NCG	Nonlinear Conjugate Gradients
GS	Nonlinear Gauss-Seidel/multiplicative Schwarz sweeps
FAS	Full approximation scheme (nonlinear multigrid)
MS	Multi-stage smoothers, often used with FAS for hyperbolic problems
Shell	Your method, often used as a (nonlinear) preconditioner

SNES Paradigm

SNES Interface based upon Callback Functions

- `FormFunction()`, set by `SNESSetFunction()`
- `FormJacobian()`, set by `SNESSetJacobian()`

Evaluating the nonlinear residual $F(x)$

- Solver calls the **user's** function
- User function gets application state through the `ctx` variable

PETSc *never* sees application data

SNES Function

$$F(u) = 0$$

The user provided function which calculates the nonlinear residual has signature

```
PetscErrorCode (*func)(SNES snes,
                       Vec x,Vec r,
                       void *ctx)
```

- `x` - The current solution
- `r` - The residual
- `ctx` - The user context passed to `SNESSetFunction()`
  Use this to pass application information, e.g. physical constants

SNES Jacobian

User-provided function calculating the Jacobian Matrix

```
PetscErrorCode (*func)(SNES snes,Vec x,Mat *J,Mat *M,
                       MatStructure *flag,void *ctx)
```

- `x` - The current solution
- `J` - The Jacobian
- `M` - The Jacobian preconditioning matrix (possibly J itself)
- `ctx` - The user context passed to `SNESSetFunction()`
  - Use this to pass application information, e.g. physical constants
- Possible `MatStructure` values are:
  - `SAME_NONZERO_PATTERN`
  - `DIFFERENT_NONZERO_PATTERN`

Alternatives

- a builtin sparse finite difference approximation (“coloring”)
- automatic differentiation (ADIC/ADIFOR)

Finite Difference Jacobians

PETSc can compute and explicitly store a Jacobian

- Dense
  - Activated by `-snes_fd`
  - Computed by `SNESDefaultComputeJacobian()`
- Sparse via colorings
  - Coloring is created by `MatFDColoringCreate()`
  - Computed by `SNESDefaultComputeJacobianColor()`

Also Matrix-free Newton-Krylov via 1st-order FD possible

- Activated by `-snes_mf` without preconditioning
- Activated by `-snes_mf_operator` with user-defined preconditioning
  - Uses preconditioning matrix from `SNESSetJacobian()`

Fusing Distributed Arrays and Nonlinear Solvers

Make DM known to SNES solver

```
SNESSetDM(snes,dm);
```

Attach residual evaluation routine

```
DMDASNESSetFunctionLocal(dm,INSERT_VALUES,
        (DMDASNESFunction)FormFunctionLocal,
                          &user);
```

Ready to Roll

First solver implementation completed

Uses finite-differencing to obtain Jacobian Matrix

Rather slow, but scalable!

Timestepping

Check out slides 162-168 from

`http://www.mcs.anl.gov/petsc/documentation/tutorials/BuffaloTutorial.pdf`

PETSc and GPUs

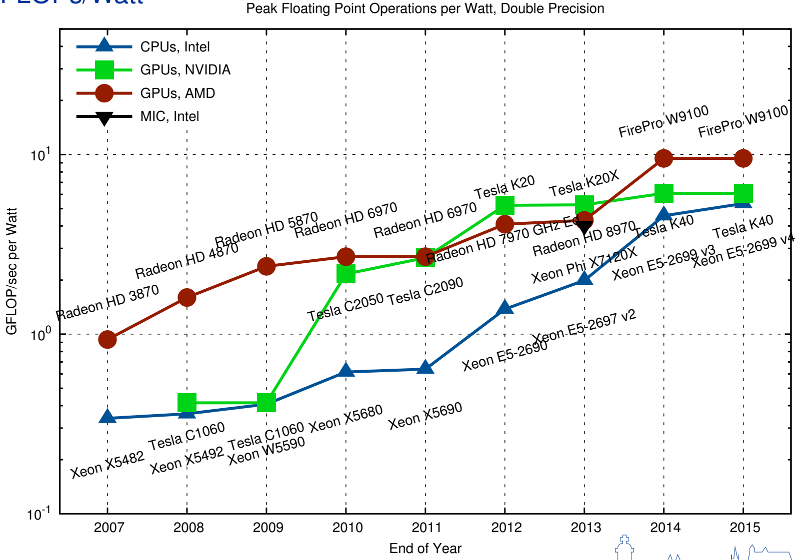
Why bother?

Don't believe anything
unless you can run it

Matt Knepley

Why bother?

GFLOPs/Watt



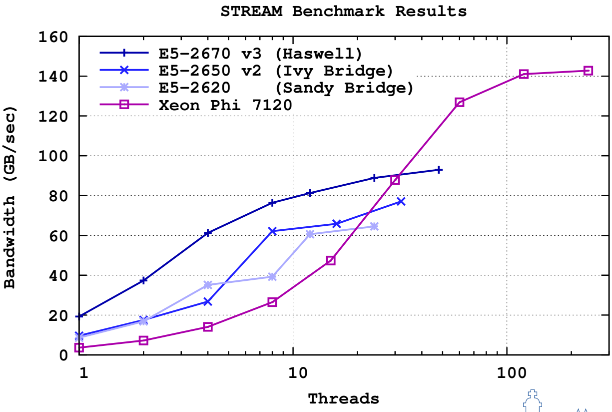
Why bother?

Procurements

Theta (ANL, 2016): 2nd generation INTEL Xeon Phi

Summit (ORNL, 2017), Sierra (LLNL, 2017): NVIDIA Volta GPU

Aurora (ANL, 2018): 3rd generation INTEL Xeon Phi



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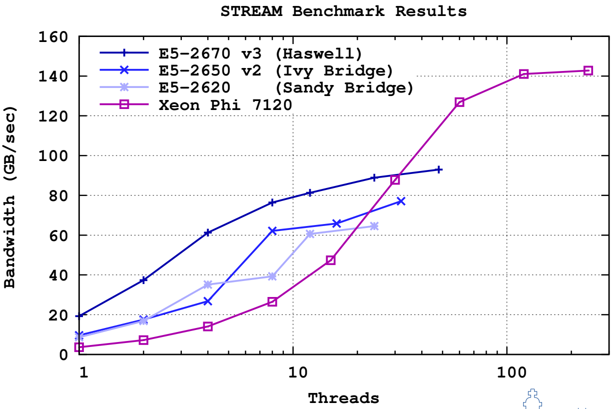


PETSc on GPUs and MIC:

Current Status

Available Options

Native on Xeon Phi

Cross-compile for Xeon Phi

CUDA

CUDA-support through CUSP

`-vec_type cusp -mat_type aijcusp`

Only for NVIDIA GPUs

OpenCL

OpenCL-support through ViennaCL

`-vec_type viennacl -mat_type aijviennacl`

OpenCL on Xeon Phi very poor

Configuration

CUDA (CUSP)

CUDA-enabled configuration (minimum)

```
./configure [..] --with-cuda=1
  --with-cusp=1 --with-cusp-dir=/path/to/cusp
```

Customization:

```
  --with-cudac=/path/to/cuda/bin/nvcc
  --with-cuda-arch=sm_20
```

OpenCL (ViennaCL)

OpenCL-enabled configuration

```
./configure [..] --download-viennacl
   --with-opencl-include=/path/to/OpenCL/include
   --with-opencl-lib=/path/to/libOpenCL.so
```

How Does It Work?

Host and Device Data

```
struct _p_Vec {
  ...
  void           *data;               // host buffer
  PetscCUSPFlag valid_GPU_array;   // flag
  void           *spptr;              // device buffer
};
```

Possible Flag States

```
  typedef enum {PETSC_CUSP_UNALLOCATED,
                PETSC_CUSP_GPU,
                PETSC_CUSP_CPU,
                PETSC_CUSP_BOTH} PetscCUSPFlag;
```

How Does It Work?

Fallback-Operations on Host

Data becomes valid on host (`PETSC_CUSP_CPU`)

```
PetscErrorCode VecSetRandom_SeqCUSP_Private(..) {
  VecGetArray(...);
  // some operation on host memory
  VecRestoreArray(...);
}
```

Accelerated Operations on Device

Data becomes valid on device (`PETSC_CUSP_GPU`)

```
PetscErrorCode VecAYPX_SeqCUSP(..) {
  VecCUSPGetArrayReadWrite(...);
  // some operation on raw handles on device
  VecCUSPRestoreArrayReadWrite(...);
}
```

Example

KSP ex12 on Host

```
$> ./ex12
    -pc_type ilu -m 200 -n 200 -log_summary
```

```
KSPGMRESOrthog       228 1.0 6.2901e-01
KSPSolve               1 1.0 2.7332e+00
```

KSP ex12 on Device

```
$> ./ex12 -vec_type cusp -mat_type aijcusp
    -pc_type ilu -m 200 -n 200 -log_summary
```

```
[0]PETSC ERROR: MatSolverPackage petsc does not support
    matrix type seqaijcusp
```

Example

KSP ex12 on Host

```
$> ./ex12
    -pc_type none -m 200 -n 200 -log_summary
```

```
KSPGMRESOrthog      1630 1.0 4.5866e+00
KSPSolve               1 1.0 1.6361e+01
```

KSP ex12 on Device

```
$> ./ex12 -vec_type cusp -mat_type aijcusp
    -pc_type none -m 200 -n 200 -log_summary
```

```
MatCUSPCopyTo          1 1.0 5.6108e-02
KSPGMRESOrthog      1630 1.0 5.5989e-01
KSPSolve               1 1.0 1.0202e+00
```

Pitfalls

Pitfall: Repeated Host-Device Copies

- PCI-Express transfers kill performance
- Complete algorithm needs to run on device
- Problematic for explicit time-stepping, etc.

Pitfall: Wrong Data Sizes

- Data too small: Kernel launch latencies dominate
- Data too big: Out of memory

Pitfall: Function Pointers

- Pass CUDA function “pointers” through library boundaries?
- OpenCL: Pass kernel sources, user-data hard to pass
- Composability?

Current GPU-Functionality in PETSc

Current GPU-Functionality in PETSc

	CUSP	**ViennaCL**
Programming Model	CUDA	OpenCL
Operations	Vector, MatMult	Vector, MatMult
Matrix Formats	CSR, ELL, HYB	CSR
Preconditioners	SA-AMG, BiCGStab	-
MPI-related	Scatter	-

Additional Functionality

MatMult via cuSPARSE

OpenCL residual evaluation for PetscFE

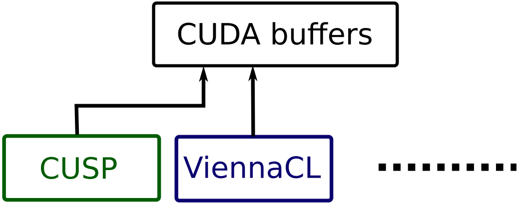
PETSc on GPUs and MIC:

Future Directions

Future: CUDA

Split CUDA-buffers from CUSP

- Vector operations by cuBLAS
- MatMult by different packages
- CUSP (and others) provides add-on functionality



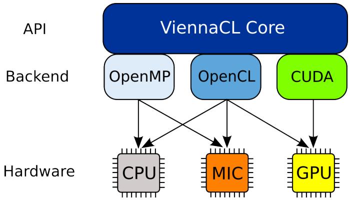
More CUSP Functionality in PETSc

- Relaxations (Gauss-Seidel, SOR)
- Polynomial preconditioners
- Approximate inverses

Future: PETSc + ViennaCL

ViennaCL

- CUDA, OpenCL, OpenMP backends
- Backend switch at **runtime**
- Only OpenCL exposed in PETSc
- Focus on shared memory machines



Recent Advances

- Pipelined Krylov solvers
- Fast sparse matrix-vector products
- Fast sparse matrix-matrix products
- Fine-grained algebraic multigrid
- Fine-grained parallel ILU

Future: PETSc + ViennaCL

Current Use of ViennaCL in PETSc

```
$> ./ex12 -vec_type viennacl -mat_type aijviennacl ...
```

Executes on OpenCL device

Possible Future Use of ViennaCL in PETSc

```
$> ./ex12 -vec_type viennacl -mat_type aijviennacl
          -viennacl_backend openmp,cuda ...
```

Pros and Cons

Use CPU + GPU simultaneously

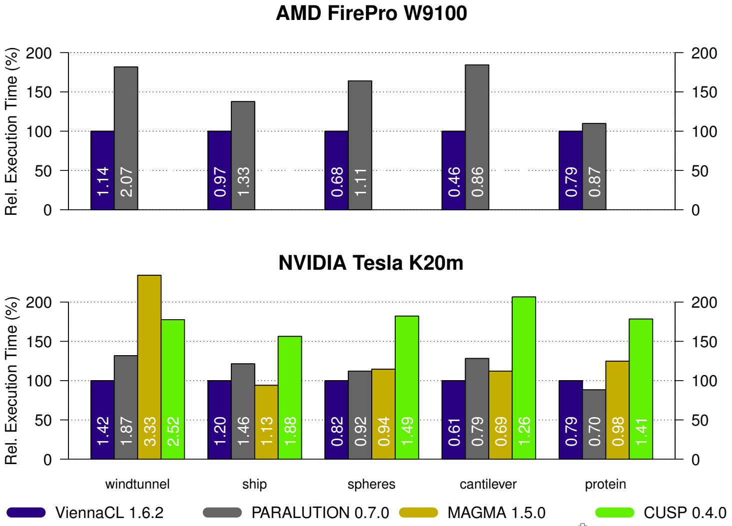
Non-intrusive, use plugin-mechanism

Non-optimal in strong-scaling limit

Gather experiences for best long-term solution

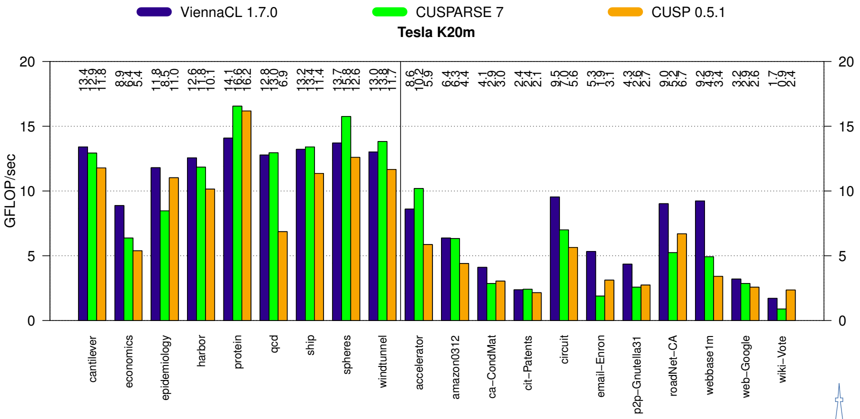
Upcoming PETSc+ViennaCL Features

Pipelined CG Method, Exec. Time per Iteration



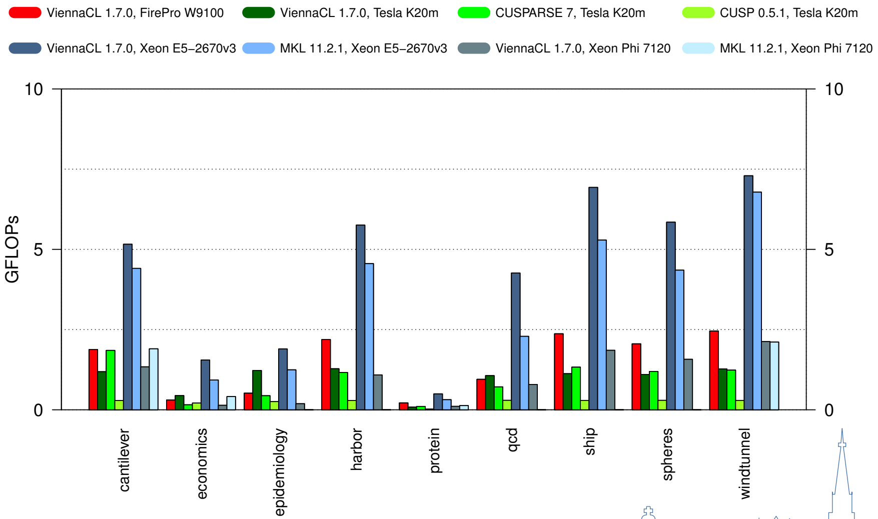
Upcoming PETSc+ViennaCL Features

Sparse Matrix-Vector Multiplication



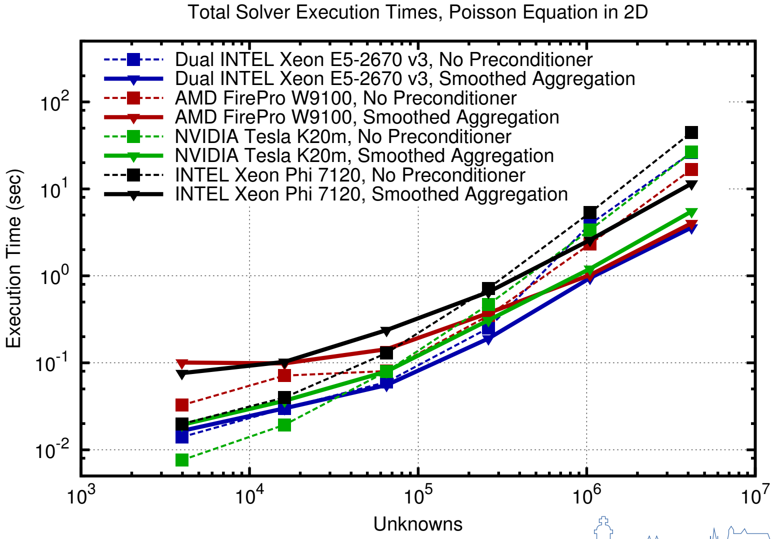
Upcoming PETSc+ViennaCL Feature

Sparse Matrix-Matrix Products

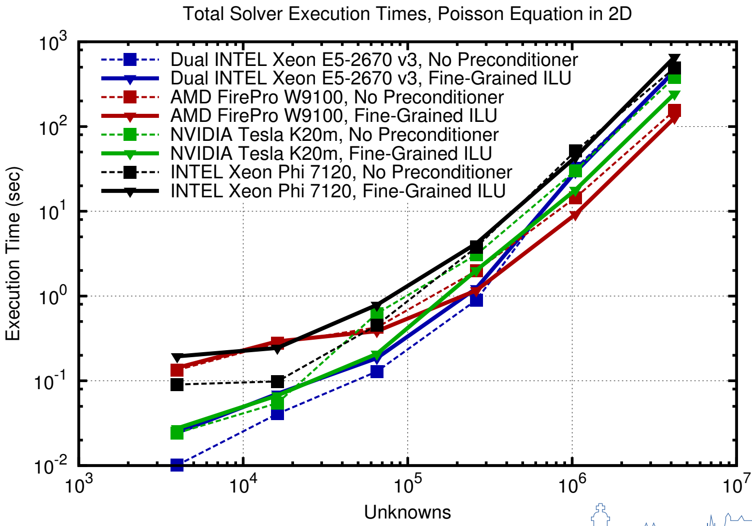


Upcoming PETSc+ViennaCL Feature

Algebraic Multigrid Preconditioners



Fine-Grained Parallel ILU (Chow and Patel, SISC, 2015)



GPU Summary and Conclusion

Currently Available

- CUSP for CUDA, ViennaCL for OpenCL
- Automatic use for vector operations and SpMV
- Smoothed Agg. AMG via CUSP

Next Steps

- Use of cuBLAS and cuSPARSE
- Better support for $n > 1$ processes
- ViennaCL as CUDA/OpenCL/OpenMP-hydra

Conclusions

PETSc can help You

- solve algebraic and DAE problems in your application area
- rapidly develop efficient parallel code, can start from examples
- develop new solution methods and data structures
- debug and analyze performance
- advice on software design, solution algorithms, and performance

  `petsc-{users,dev,maint}@mcs.anl.gov`

You can help PETSc

- report bugs and inconsistencies, or if you think there is a better way
- tell us if the documentation is inconsistent or unclear
- consider developing new algebraic methods as plugins, contribute if your idea works