Software and Performance Engineering for Iterative Eigensolvers

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High Performance Computing

project ESSEX

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Motivation 1: analyze nonlinear PDE systems

2^{nd} order PDE after space discretization

- $\mathrm{M}\dfrac{\partial\Phi}{\partial t} = \mathrm{F}(\Phi, t)$
- with suitable boundary and initial conditions

Steady state; Φ as $t \to \infty$.
Standard technique: time stepping

- may take very long
- no information about stability

physical difficulty: low frequency modes affect solution on very long time scales

Example: 3D Boussinesq equations

$$\partial u/\partial t = -\left((uu)_x + (vu)_y + (wu)_z\right) - p_x + \nu\nabla^2 u$$

$$\partial v/\partial t = -\left((uv)_x + (vv)_y + (wv)_z\right) - p_y + \nu\nabla^2 v$$

$$\partial w/\partial t = -\left((uw)_x + (vw)_y + (ww)_z\right) - p_z + \nu\nabla^2 w + g\alpha T$$

$$\partial T/\partial t = -\left((uT)_x + (vT)_y + (wT)_z\right) + \kappa\nabla^2 T$$

$$u_x + v_y + w_z = 0$$

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Our approach:

- Newton-Krylov with preconditioning
- 'parameter continuation' as globalization
- linear stability analysis $\Longrightarrow$ solve $Ax = \lambda Bx$ for some λs near 0, B spd, A not.

Example: Rayleigh-Bénard convection

- Cube-shaped domain
- heated from below
- Rayleigh-Number

$$\mathrm{Ra} = \frac{\alpha g \Delta T d^3}{\nu \kappa}$$

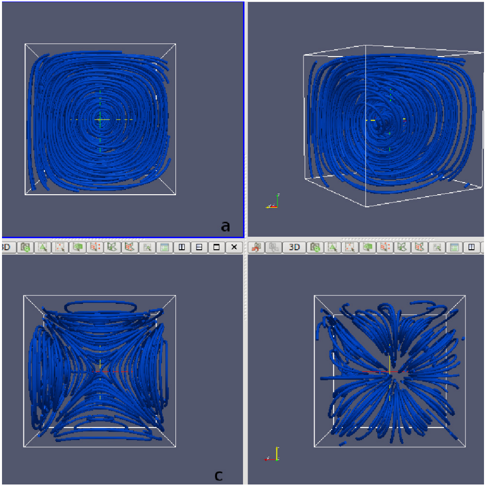


Figure: **Flow patterns near the first three primary bifurcations**
(a) x/y roll,
(b) diagonal roll,
(c) four rolls,
(d) toroidal roll

Motivation 2: provide a useful solver library

(i) **Application scientists** miss solvers that ...
- can handle generalized and non-Hermitian problems
- can be integrated deeply into applications
- can easily be used from Fortran
- support GPU accelerators and heterogenous hardware

(ii) **Numericists** need a platform for
- implementing algorithms on increasingly complex hardware
- performing meaningful performance studies

(iii) **Portability requirements:**
- easy testing and benchmarking on all levels

Jacobi-Davidson: Newton's as an Eigensolver

- Eigenvalue problem: solve $\mathrm{A}x - \lambda x = 0$ for (x, λ)
- Apply inexact Newton
- JDQR: subspace acceleration, locking and restart (Fokkema'99)

Jacobi-Davidson correction equation

- current approximation: $A\tilde{v} - \tilde{\lambda}\tilde{v} = r$,
- previously converged Schur vectors $\left(q_1, \ldots, q_k\right) = Q$
- solve approximately $(A - \tilde{\lambda}I)\Delta v = -r, \Delta v \perp \tilde{Q} = (Q, \tilde{v})$
- use some steps of preconditioned GMRES

Implementation: `https://bitbucket.org/essex/phist`

Block JDQR

outer loop: work on n_b Ritz values $\tilde{\lambda}_j$ at a time
Inner solver: compute $t_j \perp \tilde{Q}$

without preconditioning:

$$P(A - \tilde{\lambda}_j I)t_j = -r_j$$
$$P = (I - \tilde{Q}\tilde{Q}^T)$$

with (left) preconditioning,

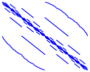
$$P_K K^{-1}(A - \tilde{\lambda}_j I)t_j = -P_K K^{-1} r_j$$
$$P_K = (I - \tilde{Q}_K(\tilde{Q}^T \tilde{Q}_K)^{-1}\tilde{Q}^T)$$

where K is a preconditioner for $A - \bar{\lambda} I$
and $\tilde{Q}_K = K^{-1}\tilde{Q}$.

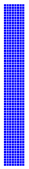
blocked solvers: separate Krylov spaces, but using block kernels.
outer loop: orthogonalize t_j against $[Q, V]$, expand V.

Common operations of iterative methods

1. Memory-bounded linear operations involving



sparse matrices
$\mathbf{A} \in \mathbb{R}^{N \times N}$ (sparseMat)



multi-vectors
$X, Y \in \mathbb{R}^{N \times m}$ (mVecs)

small and dense matrices
$C \in \mathbb{R}^{m \times k}$ (sdMats)
node-local/in *shared* memory

Developed in ESSEX/ GHOST (e.g. $Y \leftarrow \alpha AX + \beta Y$, $C \leftarrow X^T Y$, $X \leftarrow Y \cdot C$)

2. Algorithms for sdMats

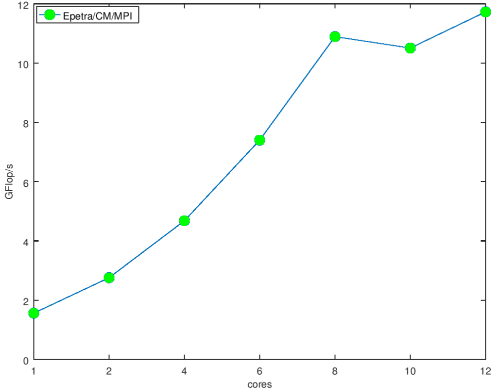
- e.g. eigendecomposition of projected matrix
- **LAPACK/PLASMA/MAGMA**

3. Sparse matrix (I)LU factorization

- not available in GHOST
- allow using external libraries via **Trilinos** interface

Why do we need our own kernels?

simple(?) operation: $C = V^T V, V \in \mathbb{R}^{1M \times 4}$



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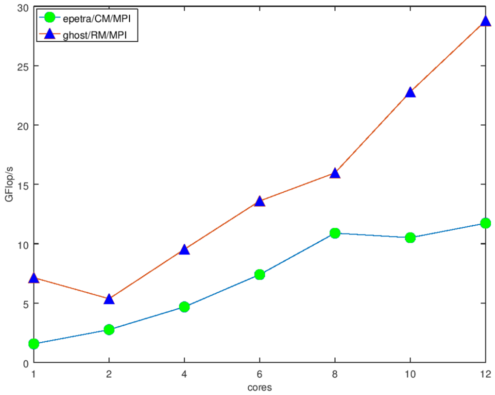

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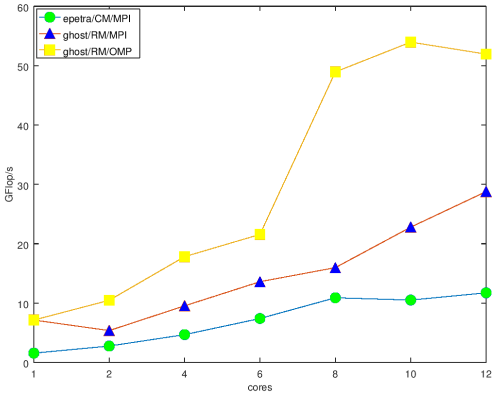

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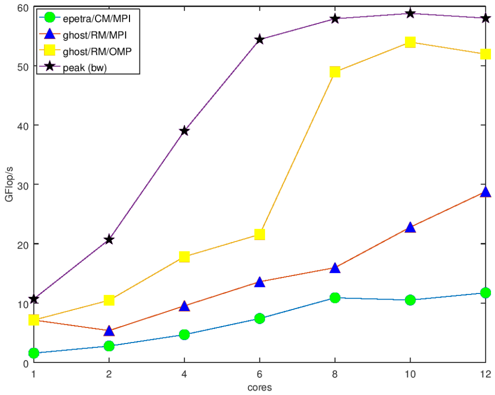
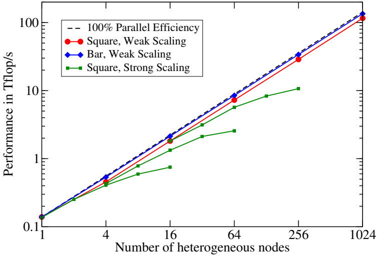


SPMD/OK Programming Model

- SPMD ('BSP') vs. task parallelism
- Heterogenous cluster: distribute problem according to limiting resource (e.g. memory bandwidth)
- **O**ptimized **K**ernels make sure each component runs as fast as possible
- User sees a simple functional interface (no general-purpose looping constructs etc.)

A success story: Chebyshev methods on Piz Daint

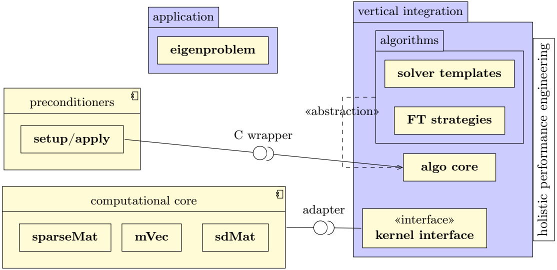


Only needs sparse matrix times multiple vector (spMMV) products and an occasional vector operation

PHIST software architecture

a Pipelined Hybrid-parallel Iterative Solver Toolkit

- facilitate algorithm development using GHOST
- holistic performance engineering
- portability and interoperability



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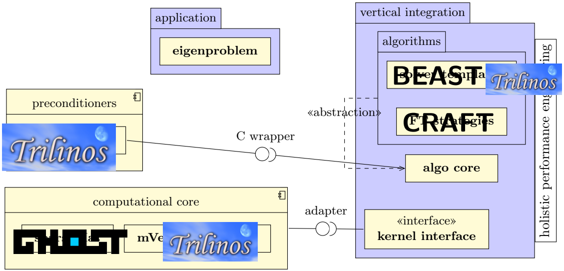

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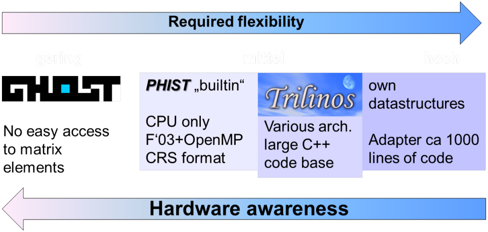
Useful abstraction: kernel interface

Choose from several 'backends' at compile time, to

- easily use **PHIST** in existing applications
- perform the same run with different kernel libraries
- compare numerical accuracy and performance
- exploit unique features of a kernel library (e.g. preconditioners)



PHIST interface example

Inspired by MPI: objects represented by handles only

C/C++:

```
// compute y = alpha*A*x + beta*y
void phist_DsparseMat_times_mvec(double alpha, phist_Dconst_sparseMat_ptr A,
        phist_Dconst_mvec_ptr x, double beta, phist_Dmvec_ptr y, int* iflag);
```

Fortran 2003:

```
subroutine phist_DsparseMat_times_mvec(alpha, A, x, beta, y, iflag)
  use iso_c_binding, only: c_double, c_ptr, c_int
  use phist_types
  real(c_double), value :: alpha, beta
  type(Dconst_sparseMat_ptr), value :: A
  type(Dconst_mvec_ptr), value :: x
  type(Dmvec_ptr), value :: y
  integer(c_int) :: iflag
```

similar **Python** interface exists

Inspired by Petra: comm, map, views

Cool features of PHIST and GHOST

Task macros: out-of-order execution of code blocks

- overlap comm. and comp.
- asynchronous checkpointing
- ...

Consistent random vectors: make **PHIST** runs comparable

- across platforms (CPU, GPU...)
- across kernel libraries
- independent of #procs, #threads

PerfCheck: print achieved roofline performance of kernels after complete run to reveal

- deficiencies of kernel lib
- implemntation issues of algorithm (strided data access etc.)

Special-purpose operations

- fused kernels, e.g. compute $Y = \alpha \mathrm{A} X + \beta Y$ *and* $Y^T X$
- highly accurate core functions, e.g. block orthogonalization in simulated quad precision

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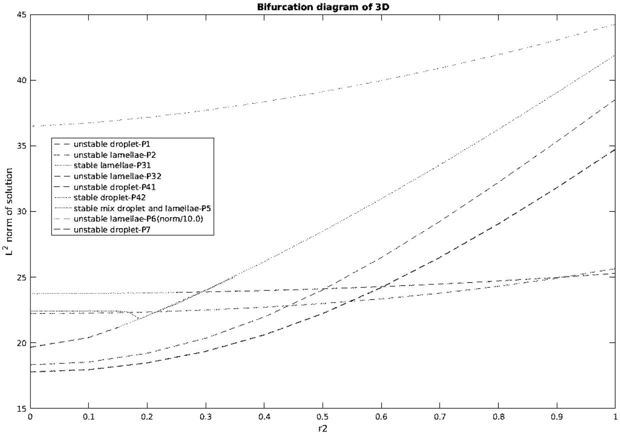
Example application: Turing problem

Reaction-Diffusion problem

$$\frac{\partial u}{\partial t} = D\delta\nabla^2 u + \alpha u(1 - r_1 v^2) + v(1 - r_2 u)$$
$$\frac{\partial v}{\partial t} = \delta\nabla^2 v + v(\beta + \alpha r_1 uv) + u(\gamma + r_2 v) \tag{1}$$

- 2D: spot and stripe patterns
- can be solved using AMG
- non-normality: JDQR + AMG fails!

3D Turing: many patterns and bifurcations



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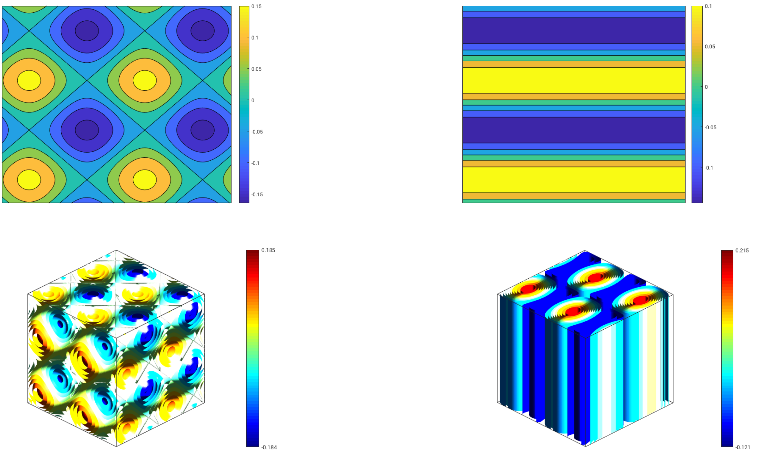
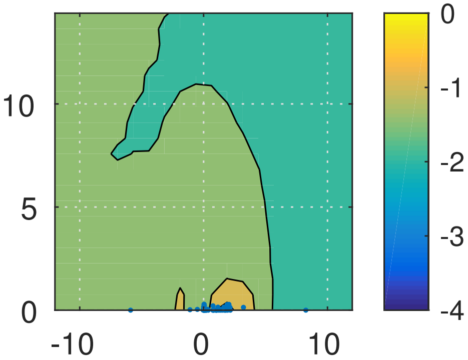


Preconditioning may be dangerous...

(normalized) projected operator $V^T P_K K^{-1} A V$ after 150 Arnoldi iterations



with 1 eigenvector of A in P_K

We used an adaptation of Trefethens Matlab code:
`http://www.cs.ox.ac.uk/pseudospectra/software.html`

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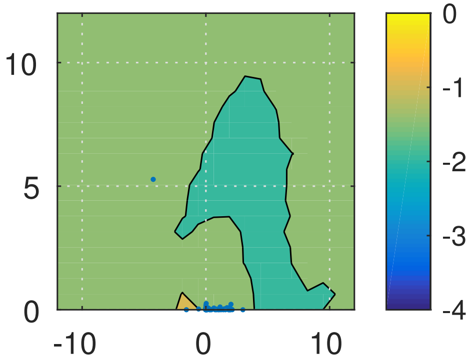

with 5x eigenvectors of A in P_K

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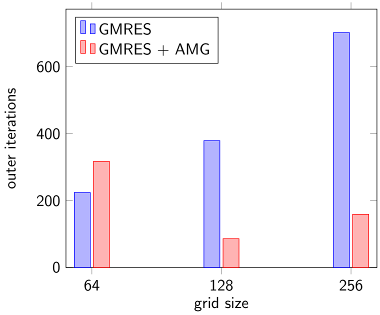
Turing with preconditioning

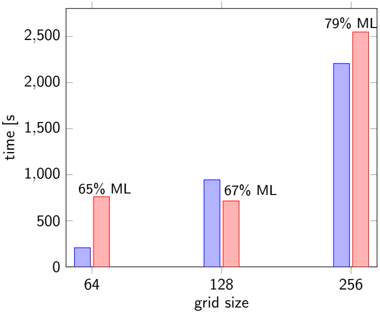
To avoid introducing non-normality by an ill-conditioned preconditioner, use AMG (ML) on the Laplacian:

Number of BJDQR(4) iterations



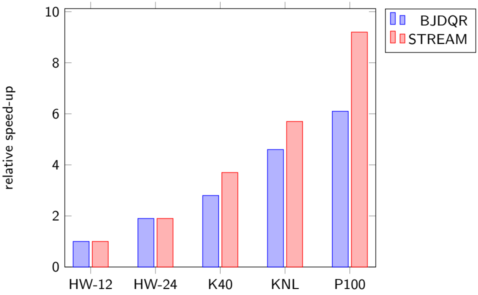
solve time

(weak scaling on 8, 64 and 512 cores)



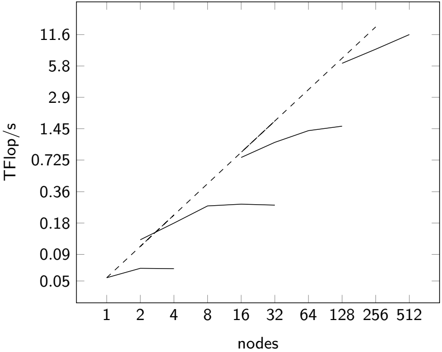
Performance portability with PHIST+GHOST

- Find 20 left-most eigenpairs of a spin-chain matrix ($N \approx 2.7M$)
- BJDQR + MINRES
- run time determined by main memory bandwidth



Scaling on Piz Daint

- 3D non-symmetric PDE problem
- block Jacobi-Davidson + GMRES
- find 10 right-most eigenvalues



It's like hungry beasts feeding from very small plates

Summary: do we provide a useful solver library?

(i) **PHIST...**

- can handle generalized and non-Hermitian problems (with caveats)
- can be integrated deeply into applications by exposing th kernel interface
- can easily be used from Fortran via Fortran bindings in phist_fort and builtin Fortran kernels
- supports GPU accelerators and heterogenous hardware via GHOST

and allows Numericists to

- implement algorithms using an abstract interface to GHOST and other libraries
- compare algorithms using the same backend
- and backends with the same algorithm

(ii) **Portable and maintainable**

- $\sim$ 10 000 test cases for kernels, core and algorithms (make test)
- perfcheck: report roofline performance of kernels after solver run

Future Work

- more memory-efficient variant for GPUs
  - do not store *AV*
  - use QMR instead of GMRES)
- more interoperability
  - e.g. apply Trilinos preconditioner to GHOST vector
- better understanding of non-Hermitian problems annd preconditioning

Questions?

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Links

- Project website

  http://blogs.fau.de/essex/
- Source code

  https://bitbucket.org/essex/

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