Karlsruhe Institute of Technology

EuroHPC Joint Undertaking

MICROCARD

Recent and upcoming developments in Ginkgo.

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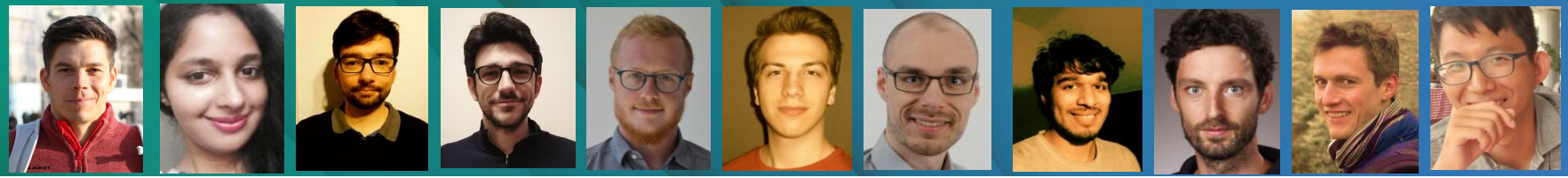
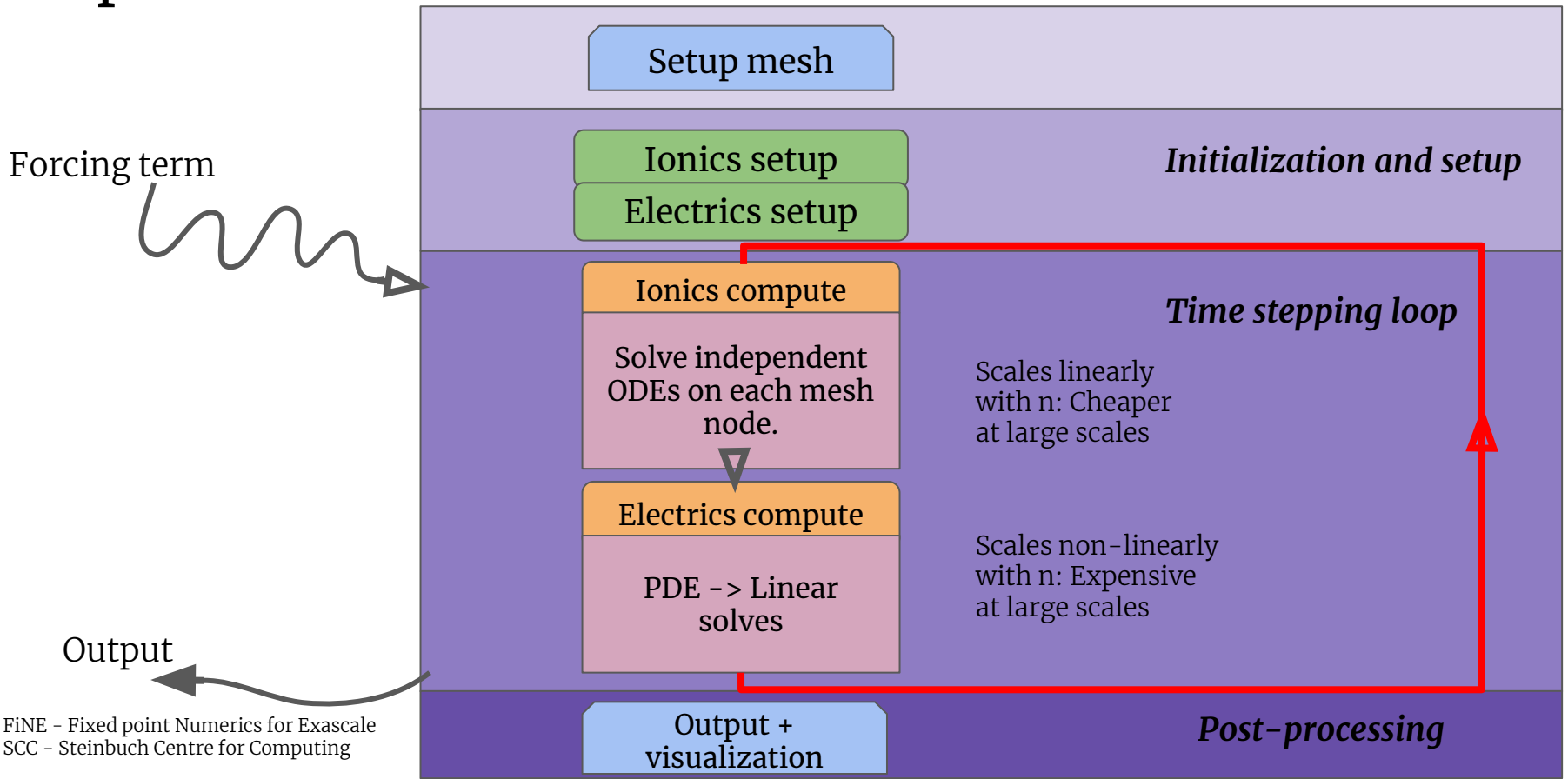
MICROCARD Workshop, Strasbourg, July 4-July 5, 2023



Outline

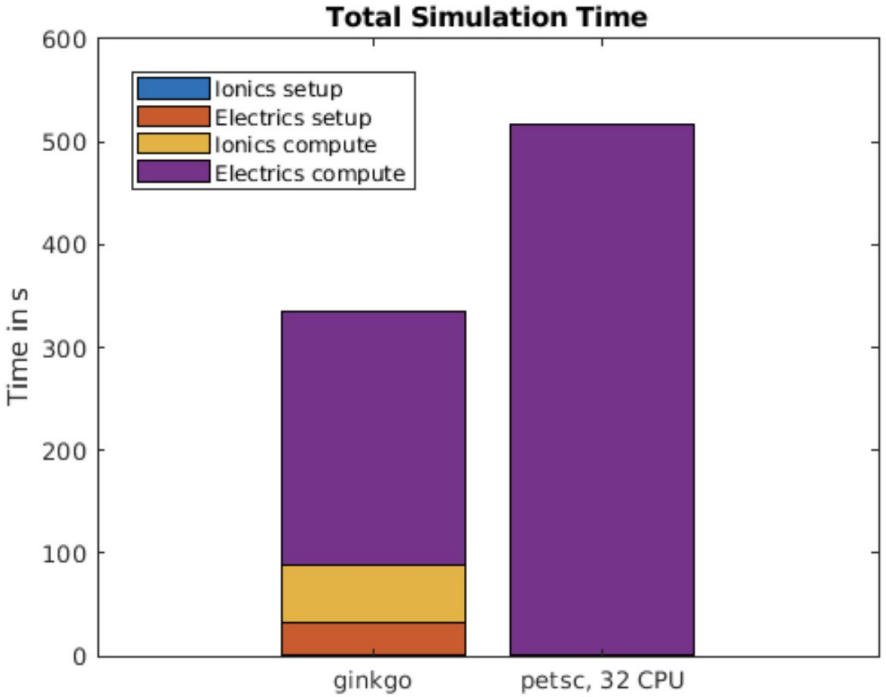
- Motivation and objectives
- Ginkgo ?
- Design philosophy and features
- A quick overview of Release 1.6.0, features and performance
- Features in development and possibly in Release 1.7.0
- Future outlook

OpenCARP simulation workflow



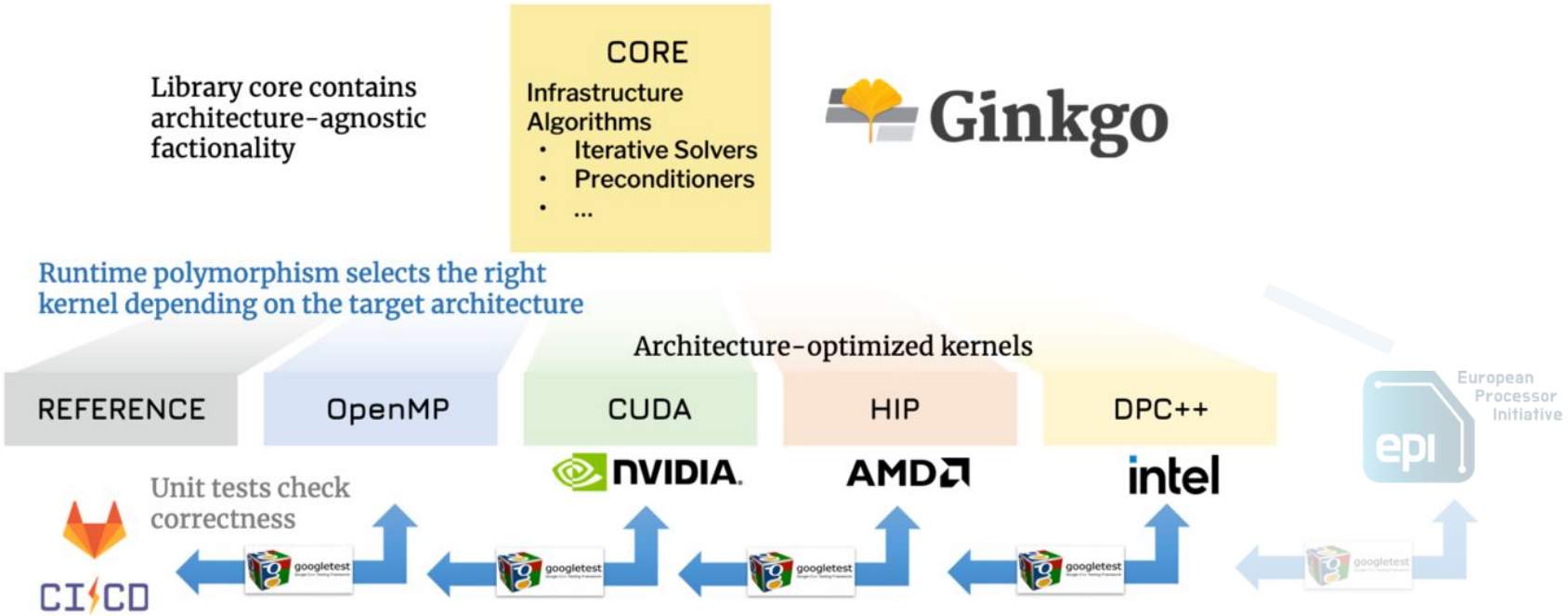
Why Ginkgo ?

- Significant part of the total time spent in linear solver.
- Crucial to optimize this bottleneck, particularly for the cell-by-cell model.
- Move computation to GPU, minimize data movement to and from GPU.

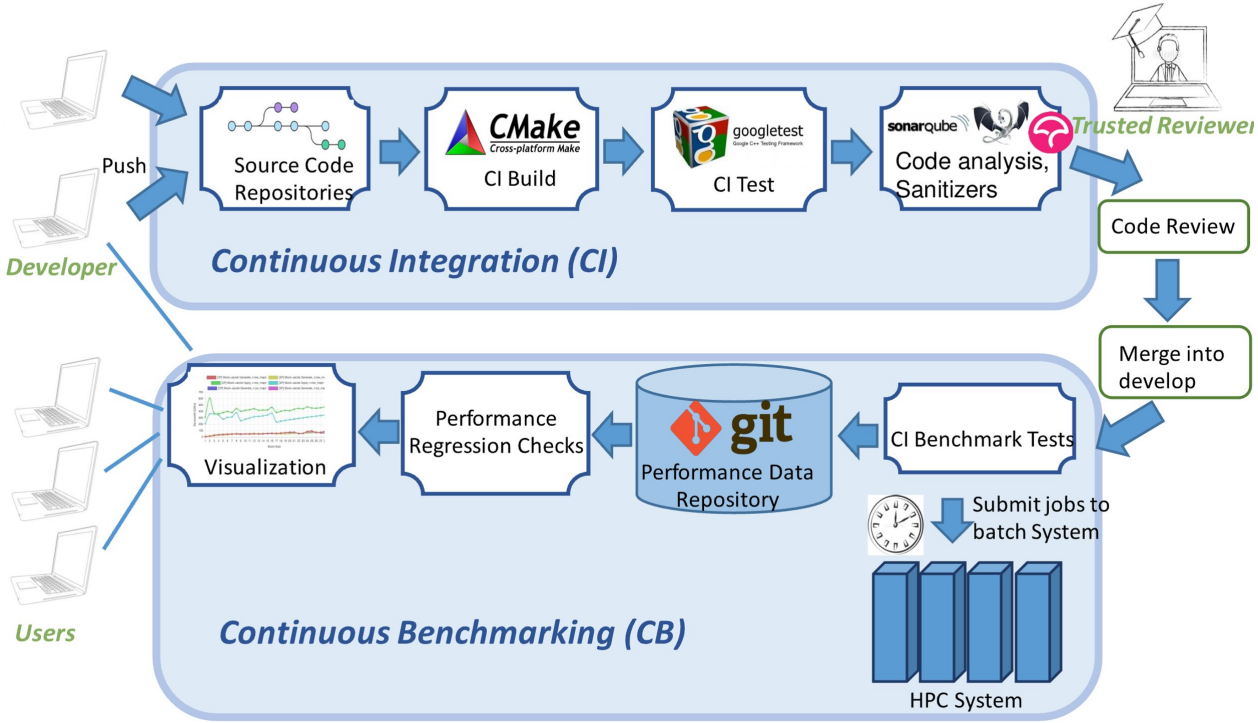


Bi-domain model: Ginkgo (1 GPU) v/s PETSc (32 CPUs)

Ginkgo: A high performance library



Ginkgo: Sustainable development



Ginkgo: Latest release - 1.6.0

- Support for sparse direct factorizations + solvers.
- Improved AMG performance.
- Profiler annotations: NVTX, ROCTX, VTune, TAU
- Stream support: Executors can now take a stream argument
- New distributed Schwarz preconditioner.
- Matrix reorderings: METIS (nested dissection), AMD (Fill-in reducing)
- Mixed precision SpMV with CSR.

More details: https://github.com/ginkgo-project/ginkgo/releases/tag/v1.6.0

Overview of features: Single executor

	Functionality	OMP	CUDA	HIP	DPC++
Basic	SpMV	✓	✓	✓	✓
	SpMM	✓	✓	✓	✓
	SpGeMM	✓	✓	✓	✓
Krylov solvers	BiCG	✓	✓	✓	✓
	BiCGSTAB	✓	✓	✓	✓
	CG	✓	✓	✓	✓
	CGS	✓	✓	✓	✓
	GMRES	✓	✓	✓	✓
	IDR	✓	✓	✓	✓
Preconditioners	(Block-)Jacobi	✓	✓	✓	✓
	ILU/IC		✓	✓	✓
	Parallel ILU/IC	✓	✓	✓	✓
	Parallel ILUT/ICT	✓	✓	✓	✓
	Sparse Approximate Inverse	✓	✓	✓	✓

	Functionality	OMP	CUDA	HIP	DPC++
AMG	AMG preconditioner	✓	✓	✓	✓
	AMG solver	✓	✓	✓	✓
	Parallel Graph Match	✓	✓	✓	✓
Sparse direct	Symbolic Cholesky	✓	✓	✓	✓
	Numeric Cholesky	✓	✓	✓	
	Symbolic LU	✓	✓	✓	✓
	Numeric LU	✓	✓	✓	
	Sparse TRSV	✓	✓	✓	
Utilities	On-Device Matrix Assembly	✓	✓	✓	✓
	MC64/RCM reordering	✓			
	Wrapping user data	✓			
	Logging	✓			
	PAPI counters	✓			

Overview of features: Distributed

- All crucial solvers and operations supported.
- Local block preconditioners supported through the distributed Schwarz preconditioner.
- Compose matrix formats between diagonal and off-diagonal matrices.

	Functionality	OMP	CUDA	HIP	DPC++
Basic	SpMV	✓	✓	✓	✓
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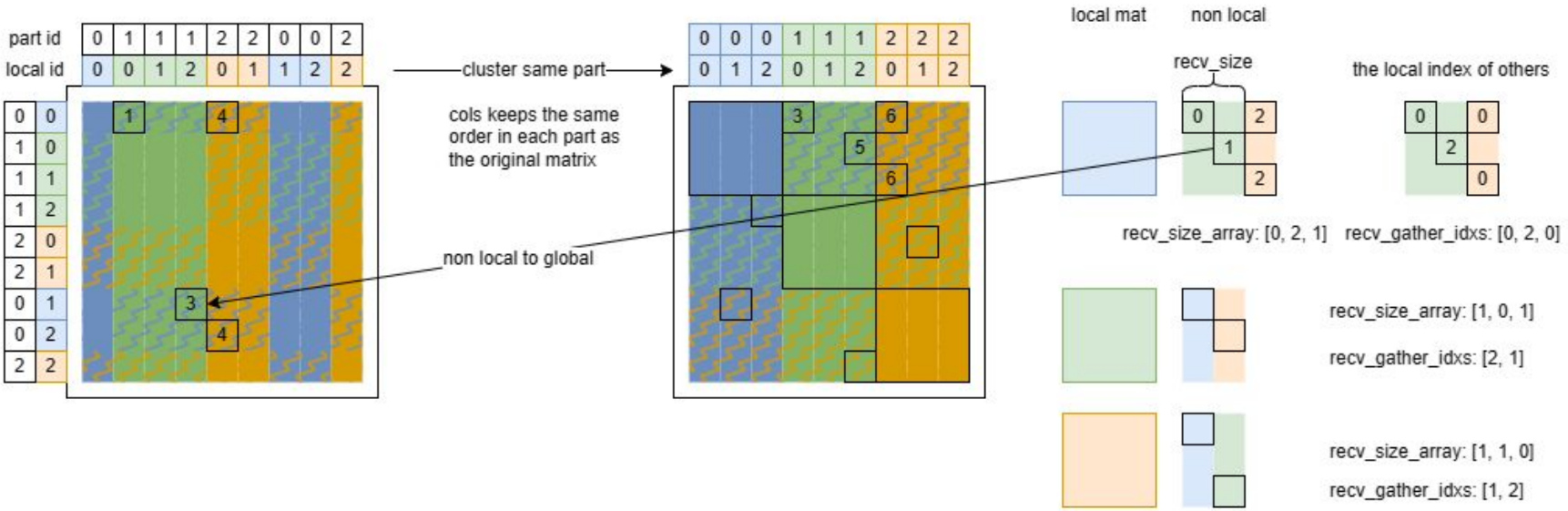
	ILU/IC		✓	✓	✓
	Parallel ILU/IC	✓	✓	✓	✓
	Parallel ILUT/ICT	✓	✓	✓	✓
	Sparse Approximate Inverse	✓	✓	✓	✓

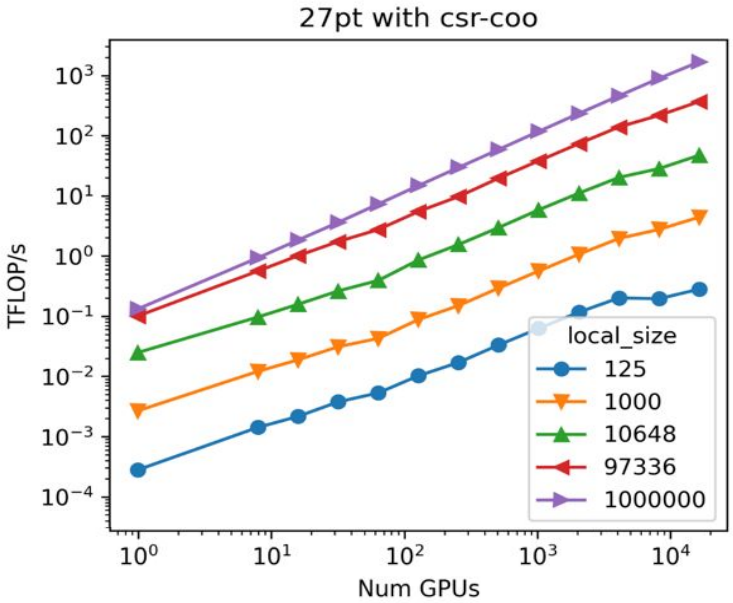
Ginkgo: Distributed data distribution

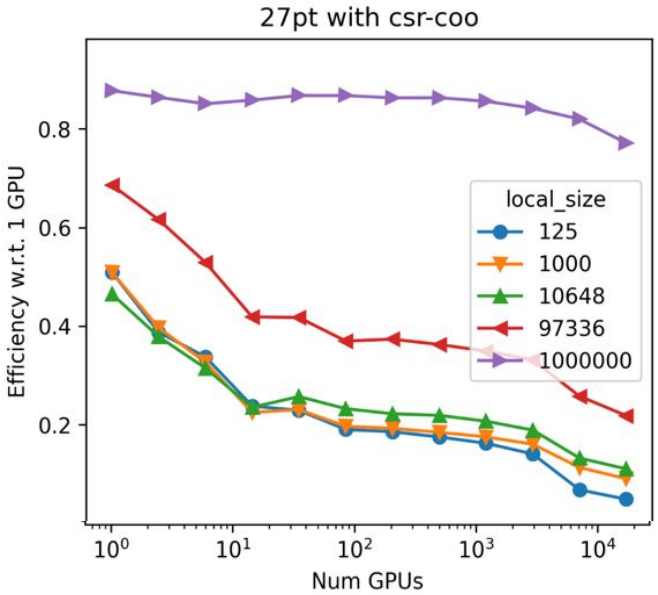


Sketch created by
Yu-Hsiang Tsai

Weak scaling: SpMV on Frontier

Cray MPICH + AMD MI250X on 16k GCDs

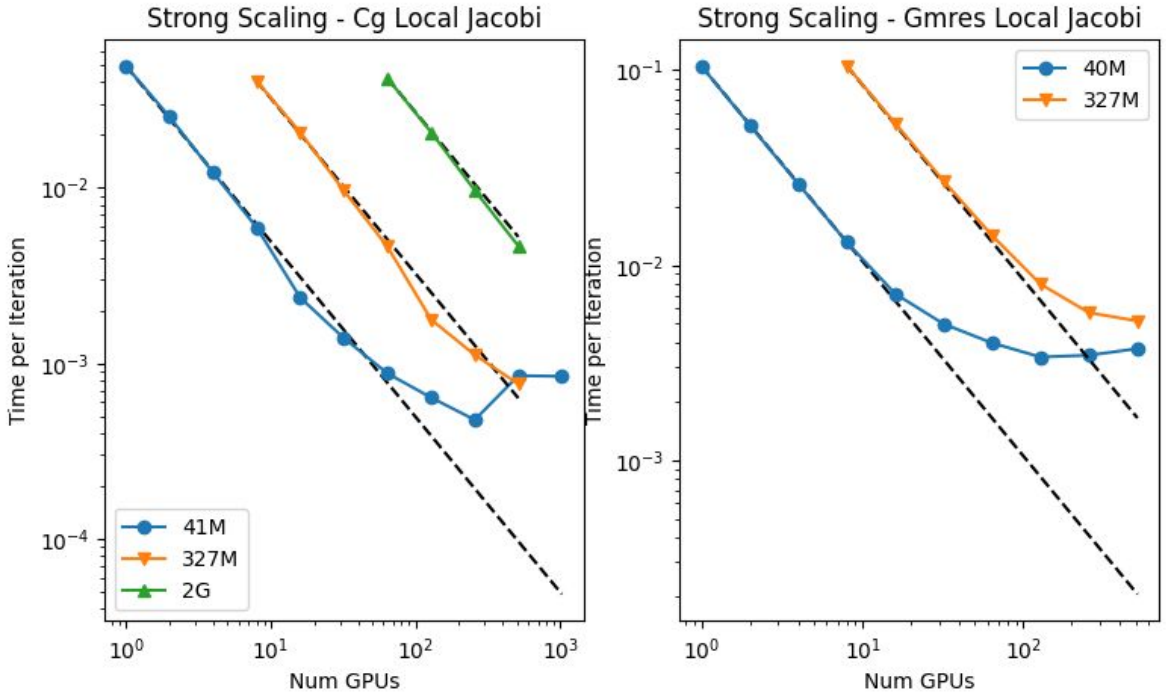




Weak scaling: problem size increases with parallel resources

Strong scaling: Solvers on Frontier

Cray MPICH + AMD MI250X

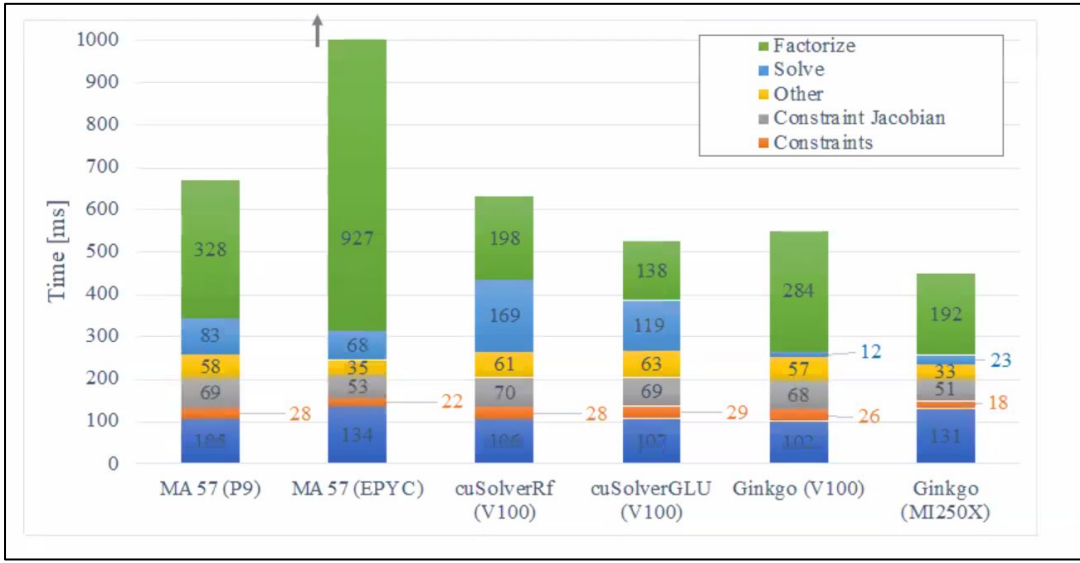


Strong scaling: constant problem size

GPU resident sparse direct solvers

- Power Grid Simulations
- All GPU solvers outperform CPU solvers
- Ginkgo first GPU-resident solver
- Enables factorization on AMD and also on Intel GPUs (No vendor alternatives available)

EXASGD



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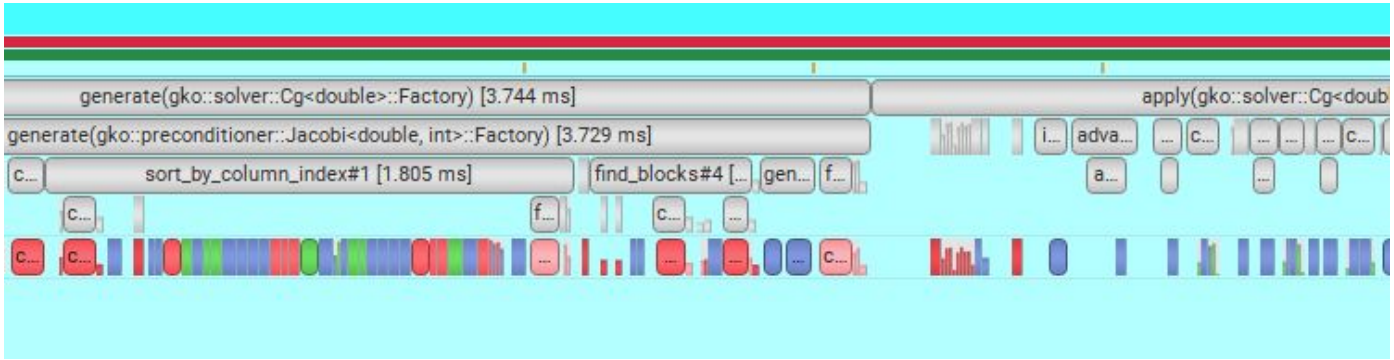
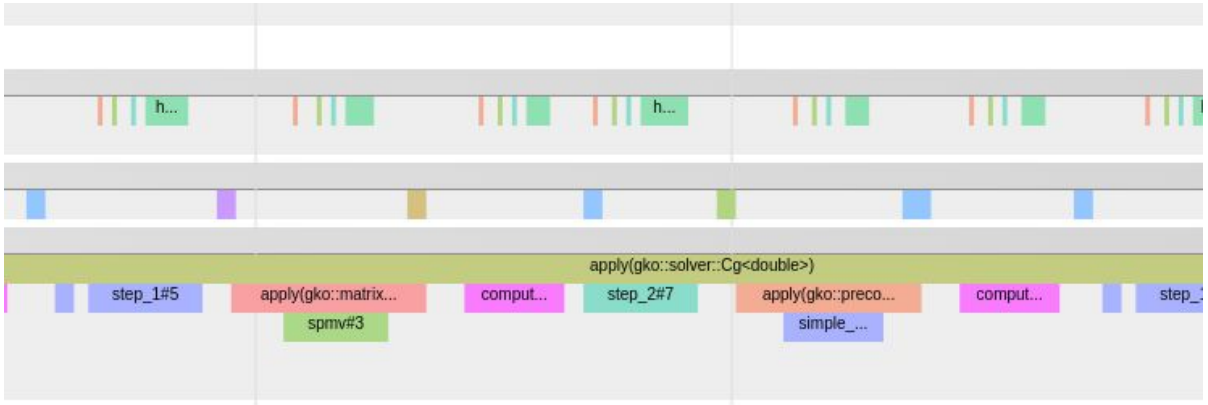
Some utilities: Profiler annotations

NVTX



ROCTX



Some utilities: Profiler annotations

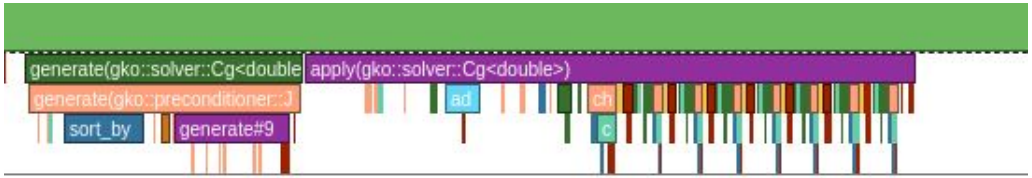
TAU

Metric: TIME
Value: Exclusive
Units: seconds

0.188	apply(gko::solver::Cg<double>)
0.098	spmv#3
0.079	apply(gko::matrix::Csr<double, int>)
0.075	apply(gko::preconditioner::Jacobi<double, int>)
0.055	compute_conj_dot#4
0.033	step_1#5
0.031	simple_apply#8
0.026	step_2#7
0.021	check(gko::stop::Iteration)
0.015	.TAU application
3.5E-4	sort_by_column_index#1
3.0E-4	generate(gko::preconditioner::Jacobi<double, int>::Factory)
3.0E-4	generate#9
1.7E-4	advanced_apply(gko::matrix::Csr<double, int>)
8.7E-5	fill_array#3
7.1E-5	aos_to_soa#2
3.9E-5	generate(gko::solver::Cg<double>::Factory)
3.9E-5	find_blocks#4
3.1E-5	advanced_spmv#5
2.5E-5	fill_in_matrix_data#2
2.5E-5	initialize#8
2.5E-5	set_all_statuses#3
2.4E-5	compute_norm2#3
1.9E-5	fill#2
1.5E-5	convert_idxs_to_ptrs#4

Tuning and Analysis Utilities

Intel VTune

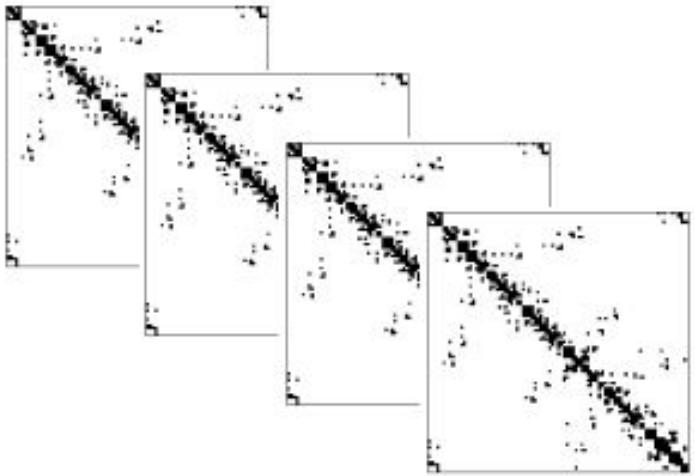


What's in development and maybe in 1.7.0 ?

- Batched iterative methods.
- More distributed preconditioners:
  - Distributed AMG (Coming soon)
  - Distributed BDDC (See Fritz's talk)
  - Two-level Schwarz methods.
- Easy solver configuration with JSON (already in use in openCARP)
- Local-only distributed matrix format: Abstract matrix format to describe and operate on overlapping partitions.
- Custom allocator support: Get around large allocation overheads with memory pool allocators (in applications).

Batched methods ?

- Batching: Independent computations that can be scheduled in parallel.
- Are highly suitable for GPUs and processors with many parallel computing units.
- Can maximize utilization of the GPU, due to excellent scalability.



Batched methods in Combustion

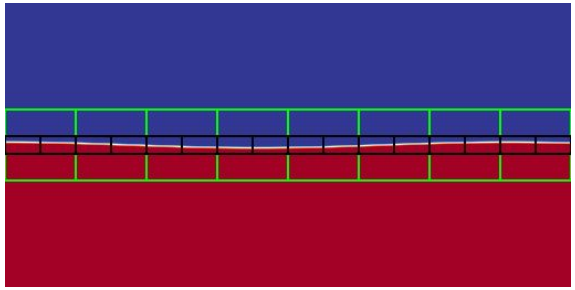
- Low mach number, non-compressible flow: leads to very stiff ODEs
- Linear multi-step time stepping with BDF

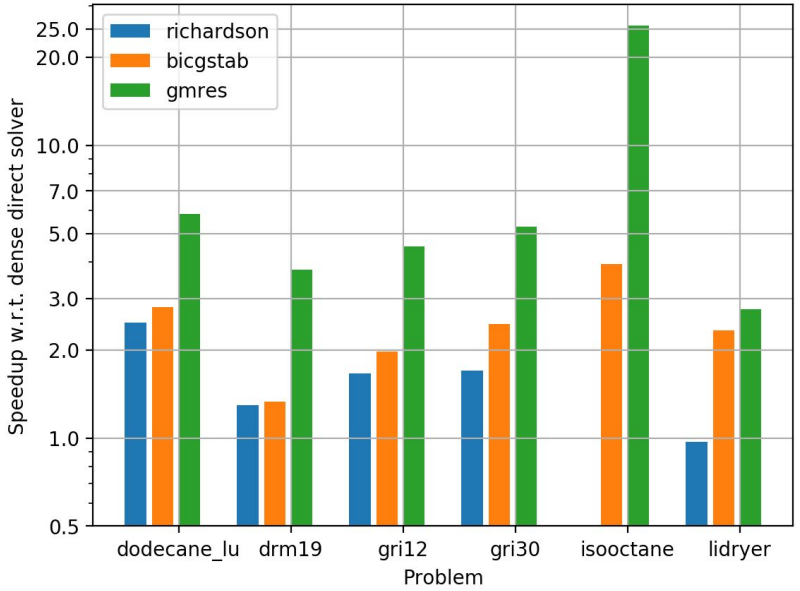
$$(I - h_n \beta_{n,0} \frac{df}{d\phi})[\phi^{n(m+1)} - \phi^{n(m)}] = -G(\phi^{n(m)})$$

- Sparsity pattern, $\mathbf{A} \equiv (I - h_n \beta_{n,0} \frac{df}{d\phi})$

  same for each cell.

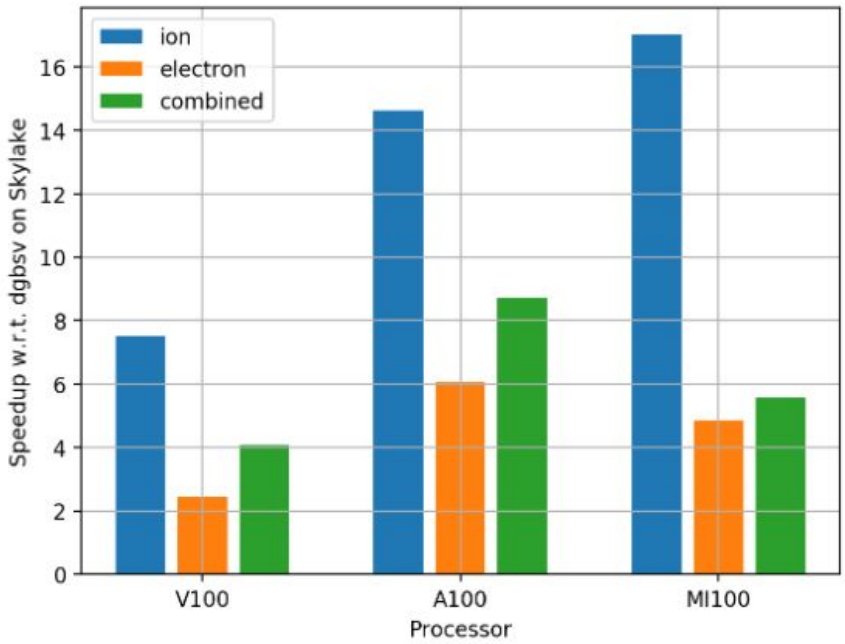
- Hence independent systems to be solved at each cell of the order of the number of cells 200k ~ 2e6 on each GPU





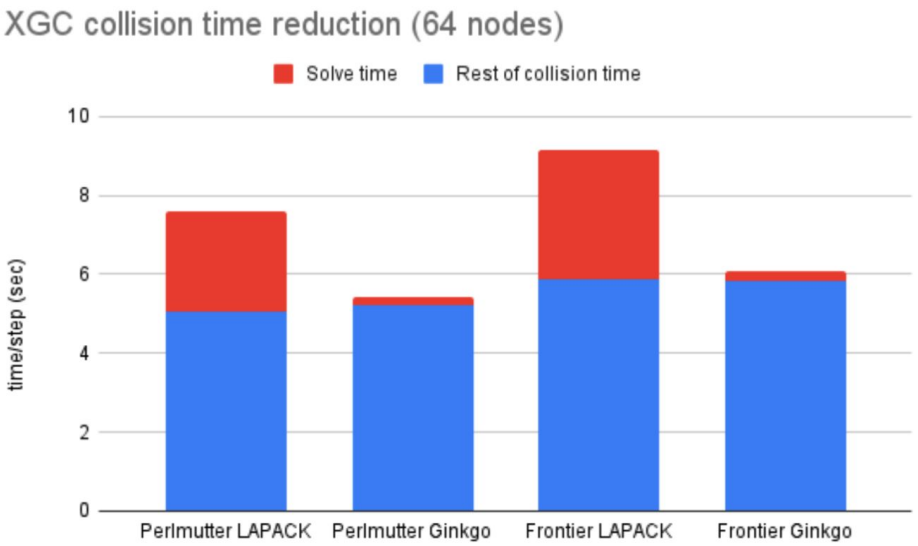
Batched methods in Fusion Plasma

- Similar idea as before, but for Particle in cell code (PIC) XGC simulating gyrokinetic plasma in a tokamak.
- Reduction in linear solve time by about 90%.
- Scales extremely well.



Batched methods in Fusion Plasma

- Similar idea as before, but for Particle in cell code (PIC) XGC simulating gyrokinetic plasma in a tokamak.
- Reduction in linear solve time by about 90%.
- Scales extremely well, due to the embarrassing parallelism.



Easy configuration for Ginkgo

- User provides a simple JSON config file at runtime.
- Solver and interface within OpenCARP configured automatically from these settings.

```
[
    {
        "name": "solver",
        "base": "CgFactory",
        "criteria": [
            {
                "name": "AbsTol",
                "base": "ResidualNormFactory",
                "baseline": "absolute",
                "reduction_factor": 1e-8
            },
            {
                "name": "Iter",
                "base": "IterationFactory",
                "max_iters": 100
            }
        ],
        "exec": "executor"
    },
    {
        "name": "precond",
        "base": "JacobiFactory",
        "max_block_size": 32,
        "exec": "executor"
    }
]
```

```
{
    "name": "precond",
    "base": "MultigridFactory",
    "criteria": [
        {
            "base": "IterationFactory",
            "max_iters": 1
        }
    ],
    "max_levels": 9,
    "min_coarse_rows": 64,
    "post_uses_pre": true,
    "zero_guess": true,
    "pre_smoother": [
        {
            "base": "IrFactory",
            "criteria": [
                {
                    "base": "IterationFactory",
                    "max_iters": 1
                }
            ],
            "solver": {
                "base": "JacobiFactory",
                "max_block_size": 1
            },
            "relaxation_factor": 0.9
        }
    ],
    "mg_level": [
        {
            "base": "AmgxPgmFactory",
            "deterministic": false
        }
    ],
    "coarsest_solver": {
        "base": "IrFactory",
```

Easy configuration for Ginkgo

```
 83  template <typename T, typename S>
 84  void ginkgo_solver<T, S>::setup_solver(abstract_matrix<T, S>& mat, double tol, int max_it, short norm,
 85                      const char* name, bool has_nullspace, void* void_logger,
 86                      const char* solver_opts_file, const char* default_opts)
 87  {
 88    using RM = gko::extension::resource_manager::ResourceManager;
 89    auto &gko_mat = dynamic_cast<ginkgo_matrix<T,S>&>(mat);
 90    auto exec = gko_mat.data->get_executor();
 91    auto non_const_exec = std::const_pointer_cast<gko::Executor>(exec);
 92    auto str_name = std::string{name} + " (Ginkgo)";
 93    this->name = str_name.c_str();
 94    this->options_file = solver_opts_file;
 95    auto logger = reinterpret_cast<opencarp::FILE_SPEC>(void_logger);
103    RM resource_manager;
104    std::ifstream options_json(this->options_file);
105    rapidjson::IStreamWrapper options_in(options_json);
106    rapidjson::Document f_options;
107    f_options.ParseStream(options_in);
108    resource_manager.insert_data<gko::Executor>("executor", non_const_exec);
109    resource_manager.read(f_options);
115
116    auto solver_factory = resource_manager.search_data<gko::LinOpFactory>("solver");
117    this->solver = solver_factory->generate(gko_mat.data);
118    dynamic_cast<gko::Preconditionable *>(this->solver.get())->set_preconditioner(this->precond);
119    this->set_stopping_criterion(normtype, tol, max_it, verbose, logger);
120  }
```

Conclusion

- Various new features available in 1.6.0
  - Distributed block preconditioners.
  - Profiling annotations.
  - Improved on on GPU AMG performance.
  - Scaling on Frontier.
- New upcoming features (1.7.0 and later)
  - Batched iterative solvers.
  - Distributed preconditioners (BDDC, AMG)
  - Easy configuration with JSON files
- Happy to discuss any additional feature requests.

Acknowledgements

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Ginkgo

https://github.com/ginkgo-project/ginkgo