A Parallel Multigrid Solver for Beam Dynamics

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Master Thesis
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14th August 2008

Outline

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Space-Charge in the Electrostatic Approximation

Whenever we have a number of moving charged particles:

- electric fields caused by Coulomb repulsion are present
- magnetic fields arising from the moving particles

Both effects acts as forces on to the particles!

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Express the Coulomb potential ϕ in terms of charge densities ρ (proportional to the particle density). The electric field can be expressed by

$$\mathbf{E} = -\nabla\phi.$$

The arising Poisson's equation for the electrostatic potential has the form

$$\nabla^2\phi = -\frac{\rho}{\varepsilon_0}.$$

The Magnetic field can be calculated from the electric field by the Lorentz transformation.

Particle-in-cell (PIC) Method in N-body Simulations

- interpolate individual particle charges to the grid
- solve the Poisson equation on the mesh in a Lorentz frame
- values of the potential at the location of individual particles is interpolated from the potential at the grid points
- typically faster $\mathcal{O}(n \log n)$ than Particle-Particle method $\mathcal{O}(n^2)$

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We apply a second order finite difference scheme which leads to a set of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

where **b** denotes the charge densities on the mesh.

Current space-charge calculation in OPAL

- FFT based direct solver: convolution with Green's function
- rectangular domain with open and periodic boundary conditions

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Goals: improvements

- solve anisotropic electrostatic Poisson PDE with an iterative solver
- irregular domain with "exact" boundary conditions

Motivation

Space-Charge Calculation in OPAL III

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- rectangular domain with open and periodic boundary conditions

Goals: improvements

- solve anisotropic electrostatic Poisson PDE with an iterative solver
- irregular domain with "exact" boundary conditions

1. implement a preconditioned iterative solver
2. incorporate this solver in OPAL
3. handle the irregular boundary points
4. investigate and implement ways to enable OPAL to use exact beam pipe geometries

Outline

Multigrid Algorithm

Mutligrid V-Cycle Algorithm

procedure MultiGridSolve(A_l, b_l, x_l, l)
if l = maxLevel-1 **then**
    DirectSolve $A_l \mathbf{x}_l = \mathbf{b}_l$
else
    $\mathbf{x}_l \leftarrow S_l^{pre}(A_l, \mathbf{b}_l, 0)$
    $\mathbf{r}_l \leftarrow \mathbf{b}_l$ - $A_l \mathbf{x}_l$ {calculate residual}
    $\mathbf{b}_{l+1} \leftarrow R_l \mathbf{r}_l$ {Restriction}
    $\mathbf{v}_{l+1} \leftarrow \mathbf{0}$
    MultiGridSolve(A_{l+1}, $\mathbf{b}_{l+1}$, $\mathbf{v}_{l+1}$, $l+1$)
    $\mathbf{x}_l \leftarrow \mathbf{x}_l$ + $P_l \mathbf{v}_{l+1}$ {coarse grid correction}
    $\mathbf{x}_l \leftarrow S_l^{post}(A_l, \mathbf{b}_l, \mathbf{x}_l)$
end if
end procedure

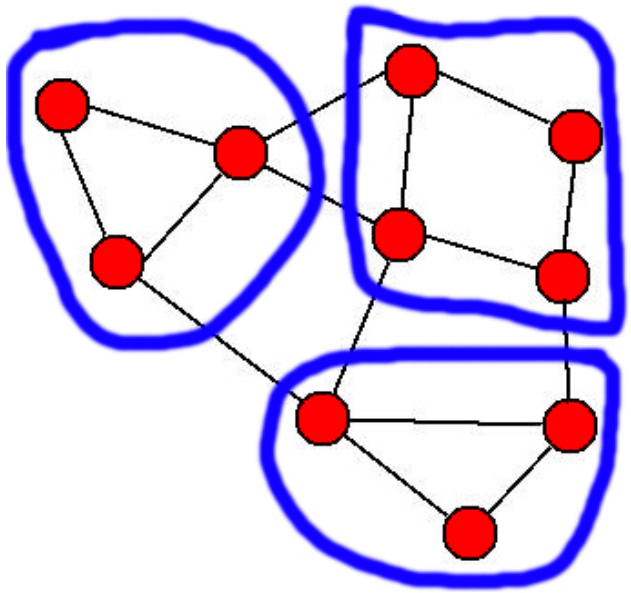
Prolongation Operator (1/2)

Smoothed Aggregation: The Grid Transfer Operator

1. discretization matrix A_l is converted into a graph G_l
2. assign each vertex of G_l is assigned to one aggregate
3. the tentative prolongation operator matrix is formed
   - matrix rows correspond to vertices
   - matrix columns to aggregates

$$p_{i,j} = \begin{cases} 1 & \text{if } i^{th} \text{ vertex in } j^{th} \text{ aggregate} \\ 0 & \text{otherwise} \end{cases}$$

4. improve robustness by smoothing the tentative prolongation operator



clustering vertices into aggregates

Prolongation Operator (2/2)

Smoothed Aggregation: Parameters

We employed a “decoupled” aggregation scheme:

- aggregates of size 3^d in d dimensions $(3 \times 3 \times 3 = 27)$
- each processor aggregate its portion of the grid
- many aggregates near inter-processor boundaries with non-optimal size
- number of processors determine number of aggregates: coarse problem may still be to big
- number of vertices is substantially reduced in every coarsening step
- typical operator complexity for decoupled aggregation is 1.5

Smoothing Operator and Coarse Level Solver

A Chebyshev polynomial smoother is used as pre- and postsmoother:

- polynomial smoothers perform well for parallel solvers (R. Tuminaro and C. Tong, 2000)
- profit of architecture optimized matrix vector products
- polynomial smoothers are easy to parallelize

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- polynomial smoothers are easy to parallelize

We chose to use a LU based solver as direct coarse level solver

Implementation (1/3)

For preconditioner setup and iterative solver we used TRILINOS:

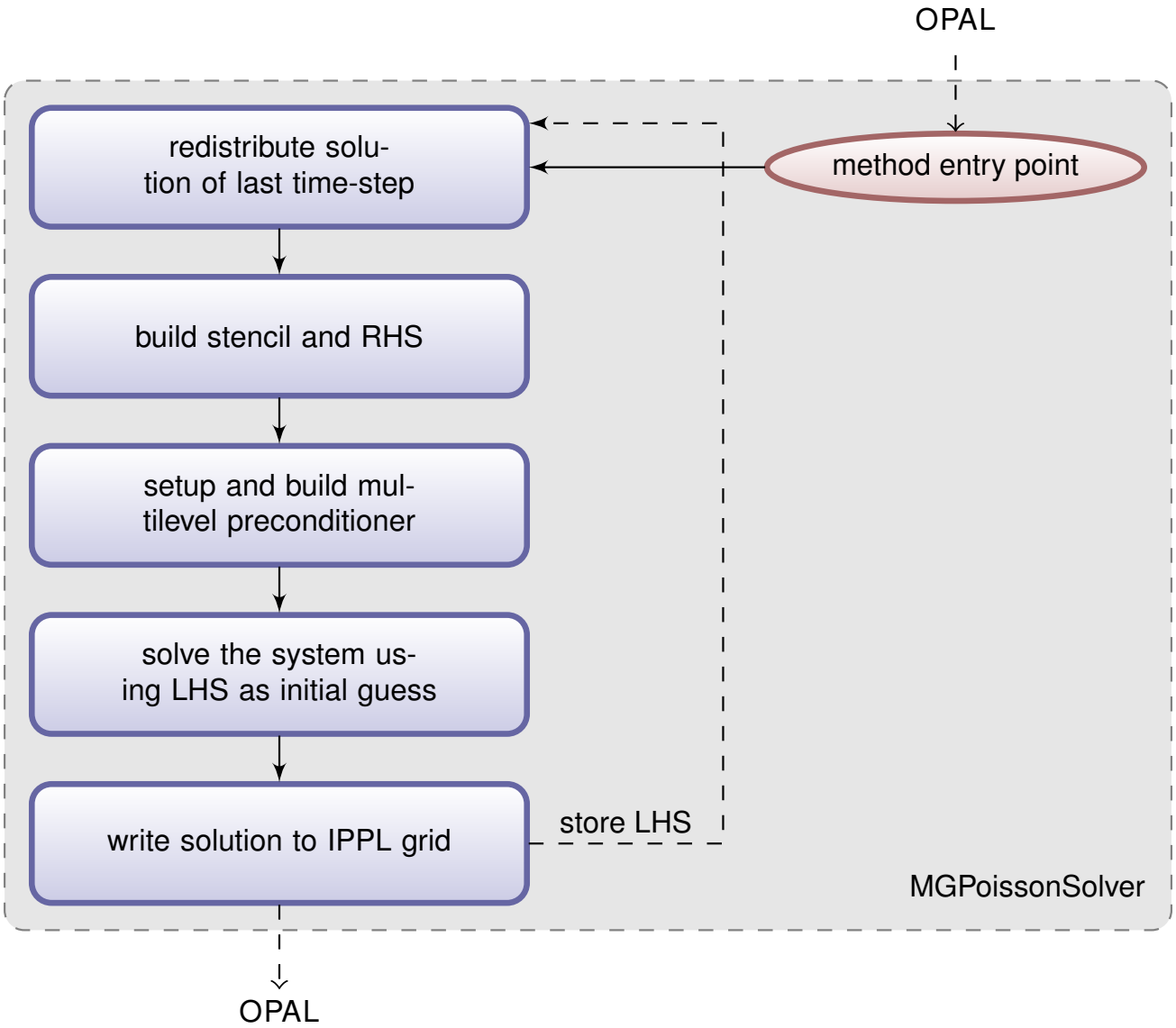
- ML: smoothed aggregation based AMG preconditioner
- EPETRA: distributed matrices and vectors
- AMESOS: direct coarse level solver
- AZTECOO: iterative solver

OPAL in conjunction with Independent Parallel Particle Layer (IPPL) offers:

- parallel fields
- particle representation
- operators on fields

Implementation (2/3)

Integration in OPAL II: Solver



Implementation (3/3)

Interface between IPPL and EPETRA

IPPL to EPETRA Map

```
1: procedure IPPLToMap3D(localidx)
2: idx ← 0
3: for all localidx.x do
4:     for all localidx.y do
5:         for all localidx.z do
6:             MyGlobalElements[idx] ← bp→getIdx(x,y,z)
7:             idx ← idx + 1
8:         end for
9:     end for
10: end for
11: return new Epetra_Map(-1, NumMyElements, &MyGlobalElements[0], 0,
    Comm)
12: end procedure
```

Outline

Boundary Condition Problem

Boundary Problem

Lets denote $\Omega \subset \mathbb{R}^3$ the simply connected computational domain and $\Gamma = \Gamma_1 \cup \Gamma_2$, the boundary of Ω ($\Gamma_1 \cap \Gamma_2 = \emptyset$). As mentioned we solve:

$$\begin{aligned} \nabla^2 \phi &= -\frac{\rho}{\epsilon_0}, \text{ in } \Omega \subset \mathbb{R}^3, \\ \phi &= 0, \text{ on } \Gamma_1 \\ \frac{\partial \phi}{\partial \vec{n}} + \frac{1}{d}\phi &= 0, \text{ on } \Gamma_2, \end{aligned}$$

with ϵ_0 denotes the dielectric constant and d is the distance of the bunches centroid to the boundary.

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1. Γ_1 is the surface of an elliptic beam-pipe
2. Γ_1 is the surface of an arbitrary beam-pipe element

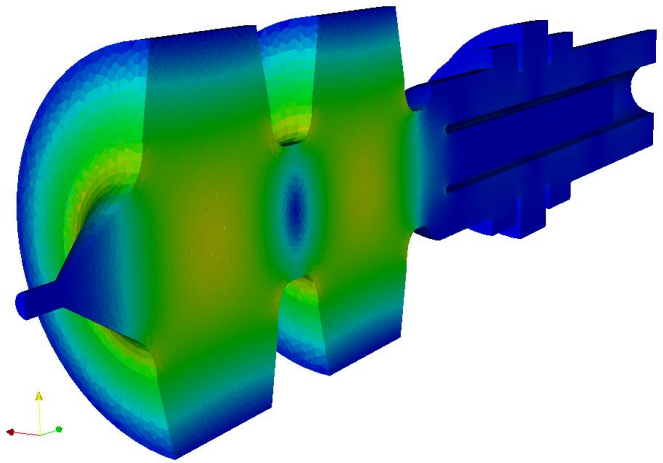
Using Real Beam-Pipe Geometries

Components

- arbitrary bounded domains are specified in files
- OPAL imports triangulated surface mesh
- efficient intersection of grid with surface mesh
- discretization approach

Motivation

- more accurate simulation of space-charges



2 Frequency LEG Cavity (Based on the design of J.-Y. Raguin (PSI))

Discretization: Irregular Domains (1/2)

$O(h)$ Approach

The key idea of this approach is to only consider grid points inside the domain neglecting the distance to the domain boundary:

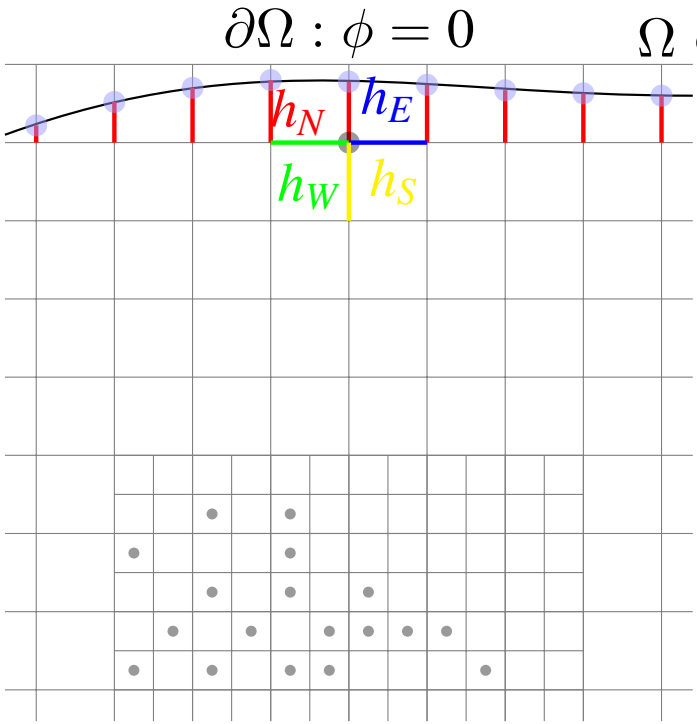
$$(h_w^{-1} + h_s^{-1} + h_e^{-1} + h_n^{-1})u_p - h_n^{-1}u_n - h_w^{-1}u_w - h_s^{-1}u_s - h_e^{-1}\underbrace{u_e}_{=0} = f_p$$

Properties

- the resulting discretization matrix is symmetric
- $O(h)$ accurate

Discretization: Irregular Domains (2/2)

Shortley-Weller approximation



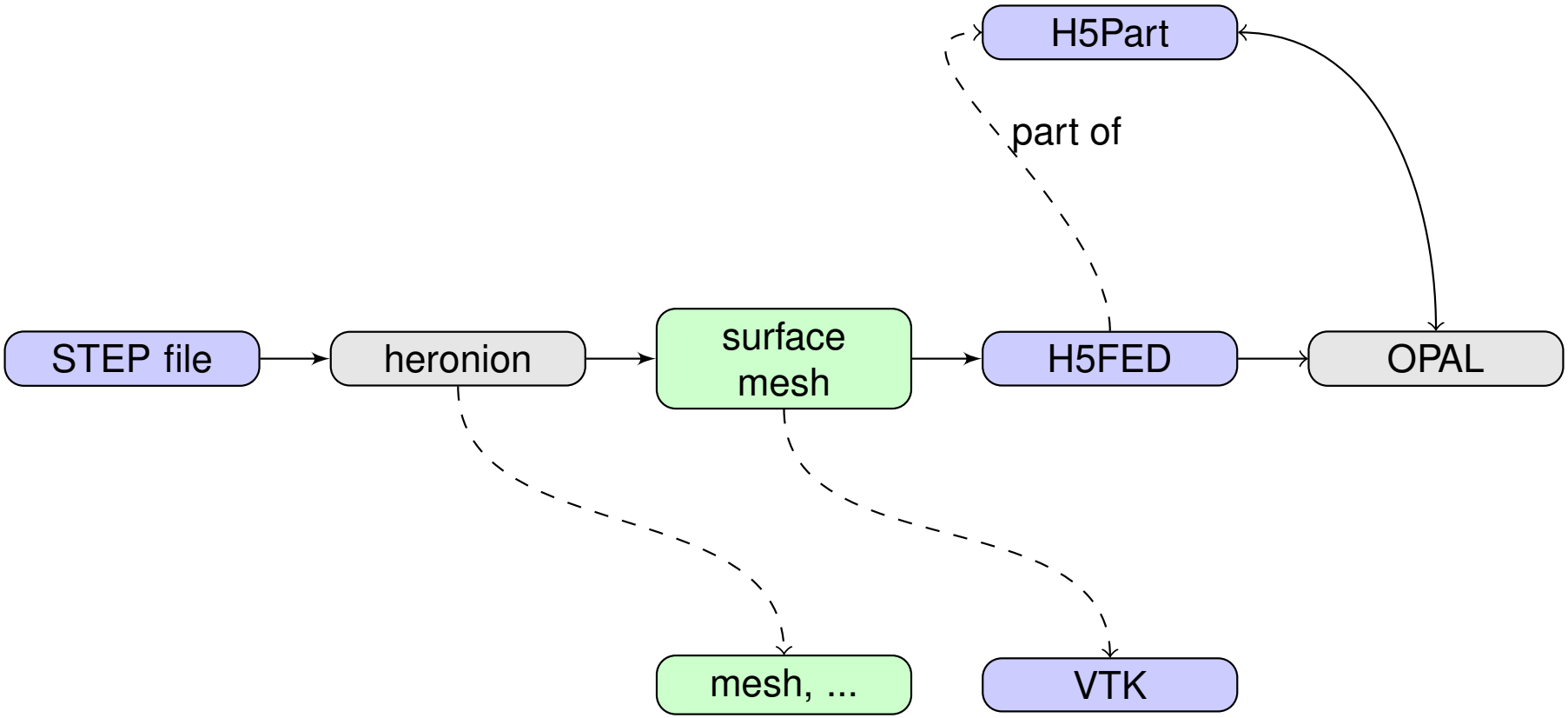
$$2 \begin{bmatrix} & \frac{b}{h_N(h_N+h_S)} & \\ \frac{a}{h_W(h_W+h_E)} & -\frac{a}{h_w h_E} - \frac{b}{h_S h_N} & \frac{a}{h_E(h_W+h_E)} \\ & \frac{b}{h_S(h_N+h_S)} & \end{bmatrix}_h$$

Properties

- the resulting discretization matrix is non-symmetric for boundary points
- $O(h^2)$ accurate

Implementation (1/2)

Importing geometries in OPAL

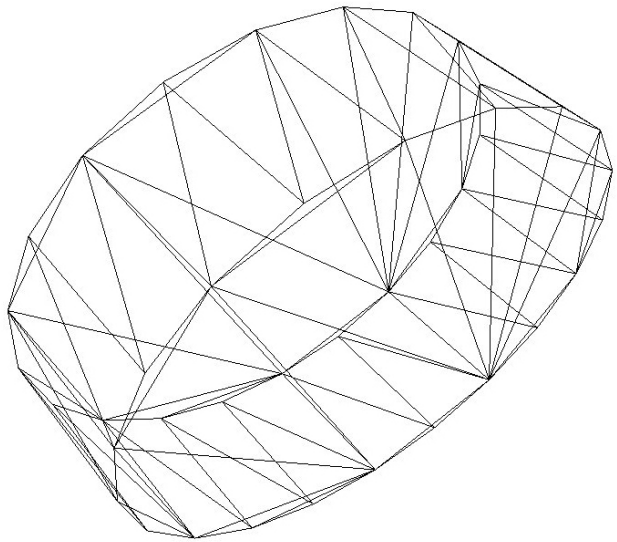


in collaboration with B. Oswald and A. Gsell (AIT)

Implementation (2/2)

Setup Phase

- extended HERONION to dump H5Fed surface mesh
- OPAL imports H5Fed files (serial): m triangles and v vertices
- efficient intersection of grid-lines with triangular surface mesh (T. Moeller and B. Trumbore (1997)):
  - arbitrary domain: $O(m(n_x + n_y + local_z))$
  - elliptic domain: $O(n_x + n_y)$
- building index table
  - arbitrary domain: $O(n_x n_y local_z)$
  - elliptic domain: $O(n_x n_y)$



Outline

Environment

Buin: Cray XT4 cluster at the CSCS in Manno

- 468 AMD dual core Opteron at 2.6 GHz
- 936 GB DDR RAM
- 30 TB Disk
- 7.6 GB/s interconnect bandwith

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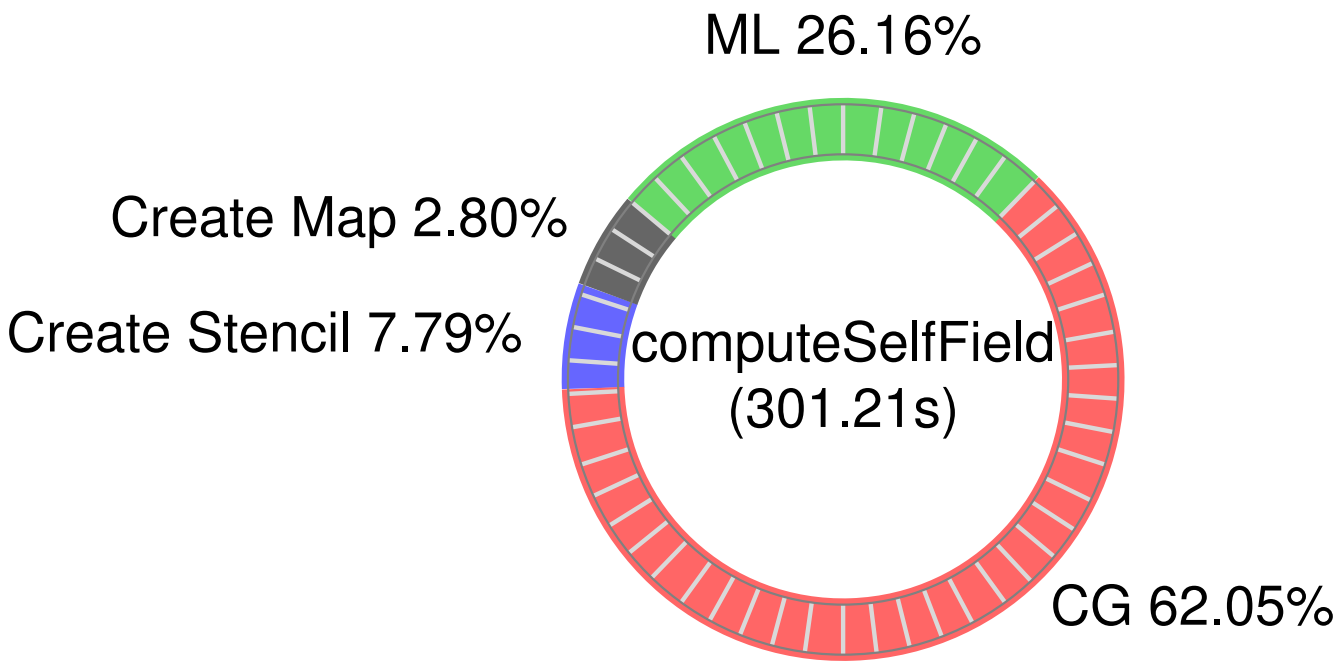

Validation

For validation purposes we defined a to the z axis, rotation symmetric potential function and calculated the analytical solution.

Arbitrary domains: tested with a triangulated surface mesh of a cylinder with the same potential function.

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Results: L_2 norms of the error:

grid size	elliptic	arbitrary
$20 \times 20 \times 20$	0.1158	0.1145
$40 \times 40 \times 40$	0.0846	0.0838
$80 \times 80 \times 80$	0.0765	0.0755

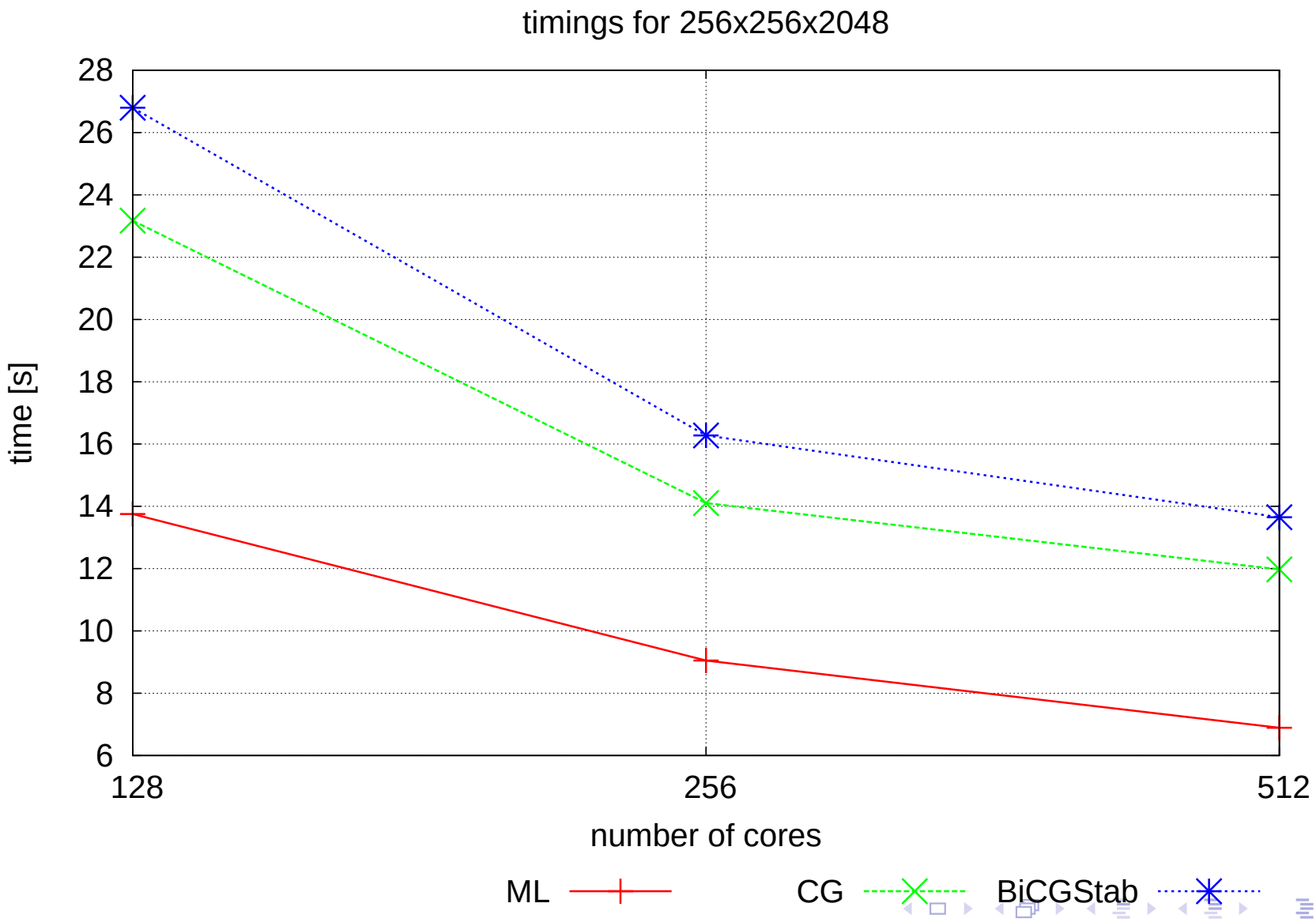
Convergence

On a $256 \times 256 \times 2048$ grid:

discretization	number of nodes	iter. for CG	iter. for BiCGStab
$O(h)$	128	12	-
$O(h)$	256	12	-
$O(h)$	512	11	-
SW	128	17	10
SW	256	17	10
SW	512	18	11

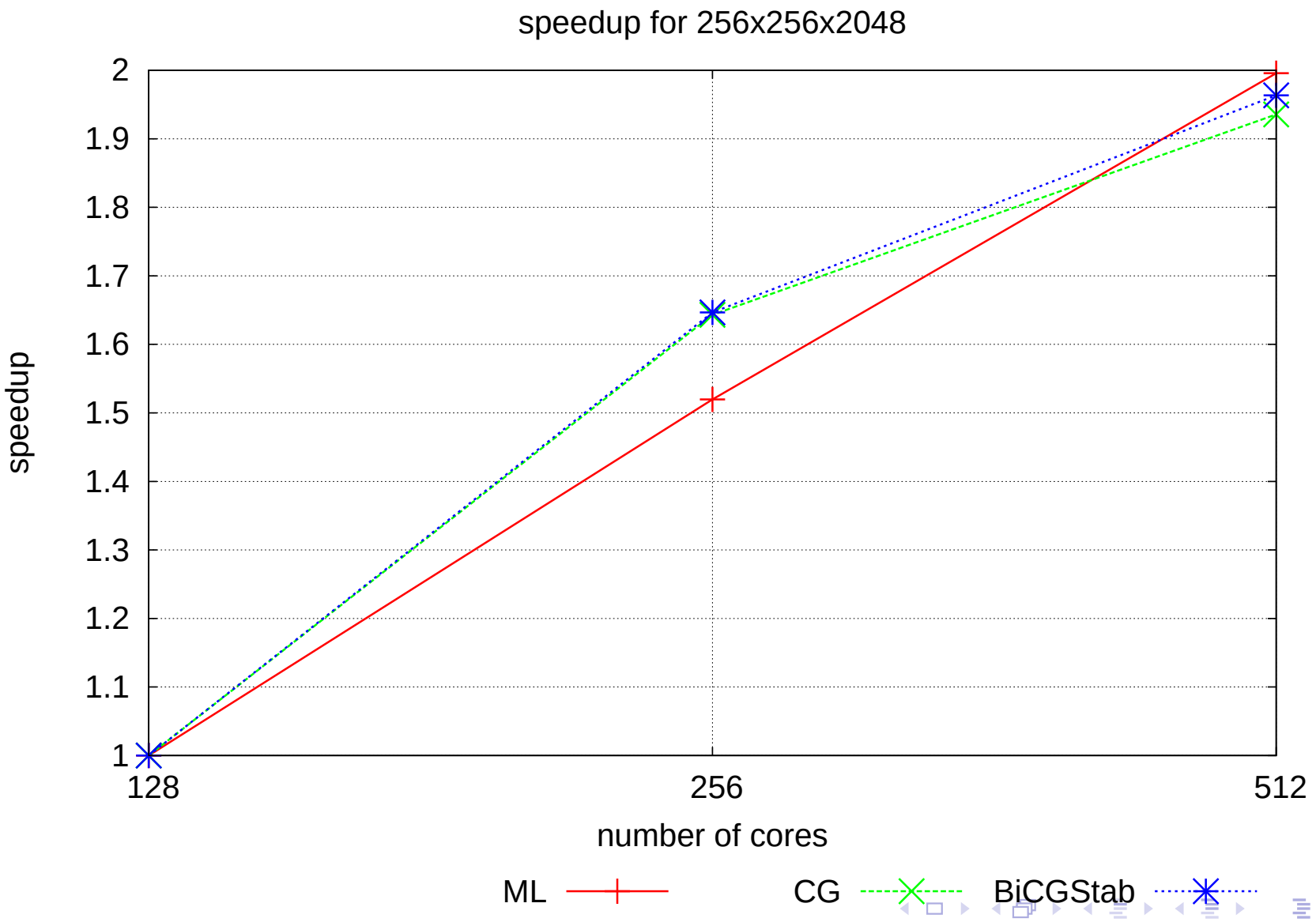
Parallel Efficiency (1/2)

Timings



Parallel Efficiency (2/2)

Speedup



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Summary

Improved Space-Charge Solver:

- is discretized with finite differences
- smoothed aggregation based algebraic Multigrid preconditioner
- fully integrated into OPAL
- reuse solutions of previous time-steps

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Improved Boundary Conditions:

- Shortley-Weller approximation
- elliptic beam-pipe domain
- arbitrary domains based on real geometries of beam-pipe elements
- beam-pipe geometries can be processed and imported

Problems and Further Work

Problems

- OPAL on Buin cluster in Manno: stand-alone solver
- ACML

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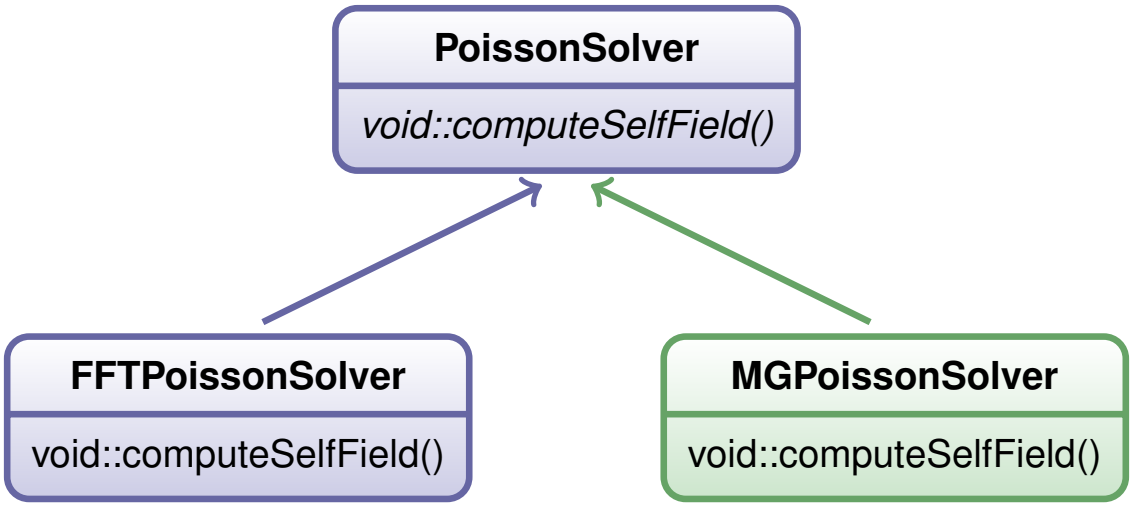
Further Work

- parallelize in x and y direction
- validation of arbitrary domains against complex geometries
- investigate in non-symmetry solver
- improve aggregation process
- adaptive mesh refinement (AMR)

Backup

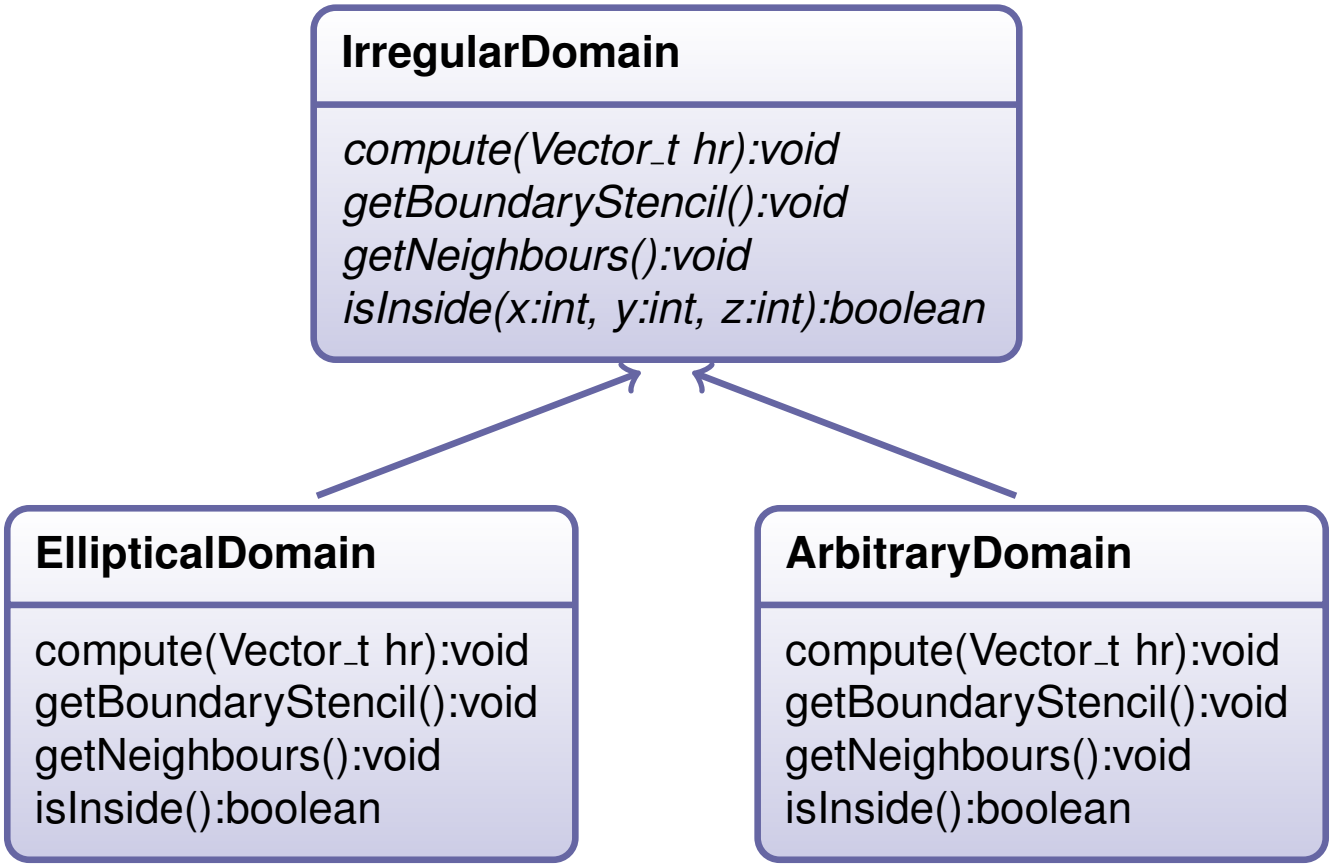
Implementation (2/4)

Integration in OPAL I: Class Hierarchy

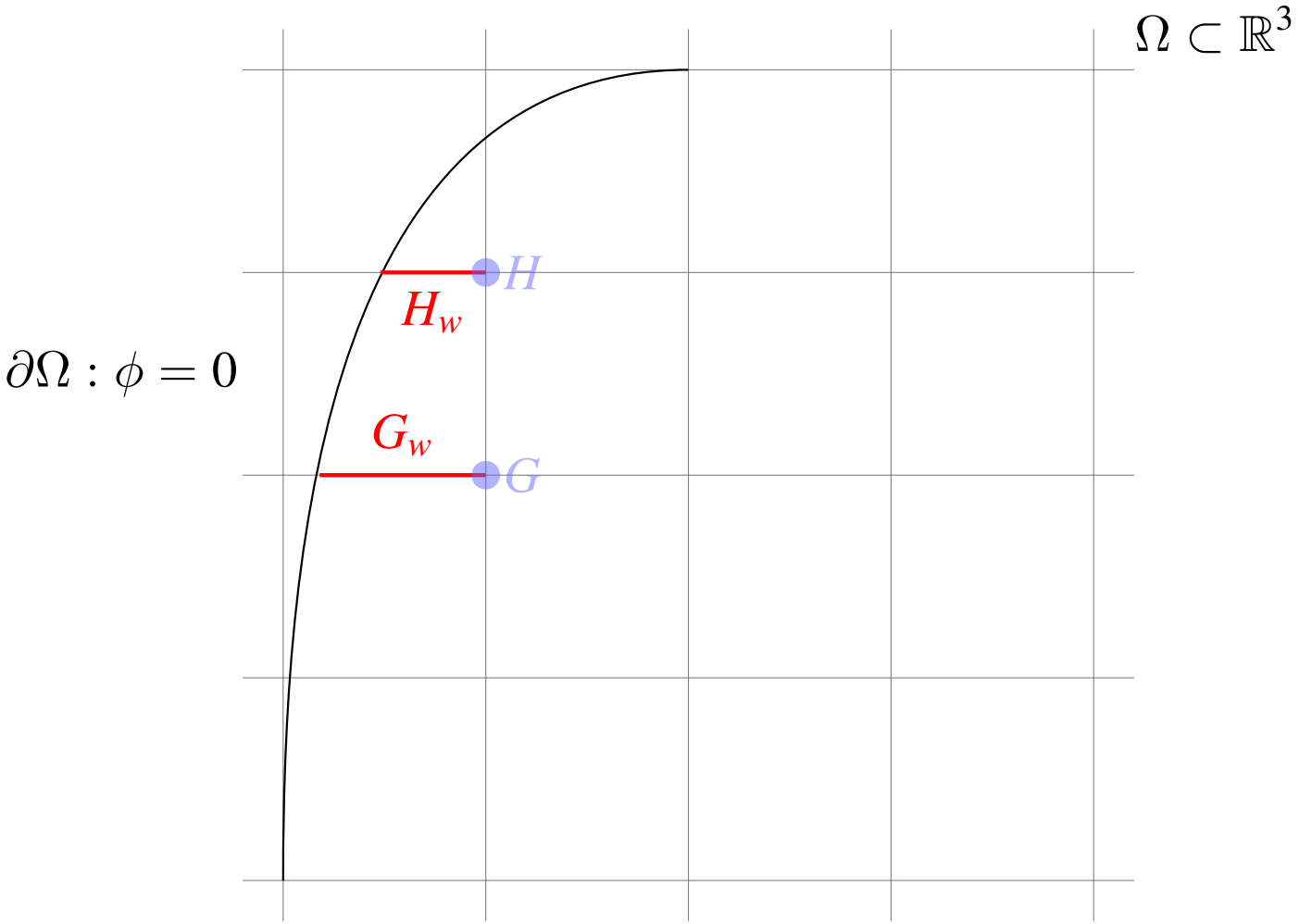


Implementation (1/3)

Class Diagram



SW: non-symmetries



Grid Operators

AMG: smoothed aggregation

Operate on directly on (linear sparse) algebraic equations:

$$\sum_j a_{ij}^h x_j^h = b_i^h$$

- replace ”grid” with ”variables”
- coarse level equations are generated without the use of any geometry
- no coarse level grids have to be generated or stored
- good preconditioner: works on all error components (in contrast to level-one preconditioner)

SA restrict operator:

$$I_H^h = (I_h - \omega D_h^{-1} A_h^f) \hat{I}_H^h$$

Multigrid Theory (1/2)

Motivation

Important Observations

- Some classical iterative methods (i.e. Gauss Seidel) have a smoothing effect on the error of any approximation for discrete elliptic problems.
- A smooth error can be well approximated on a coarse grid. This coarse grid has considerably fewer grid points and is therefore cheaper to solve.

From this two observations a Two-Grid can be deduced:

1. apply smoother
2. restrict to a grid with considerably fewer grid points (coarse)
3. solve
4. interpolate back to the fine grid
5. compute a new approximation

Multigrid Theory (2/2)

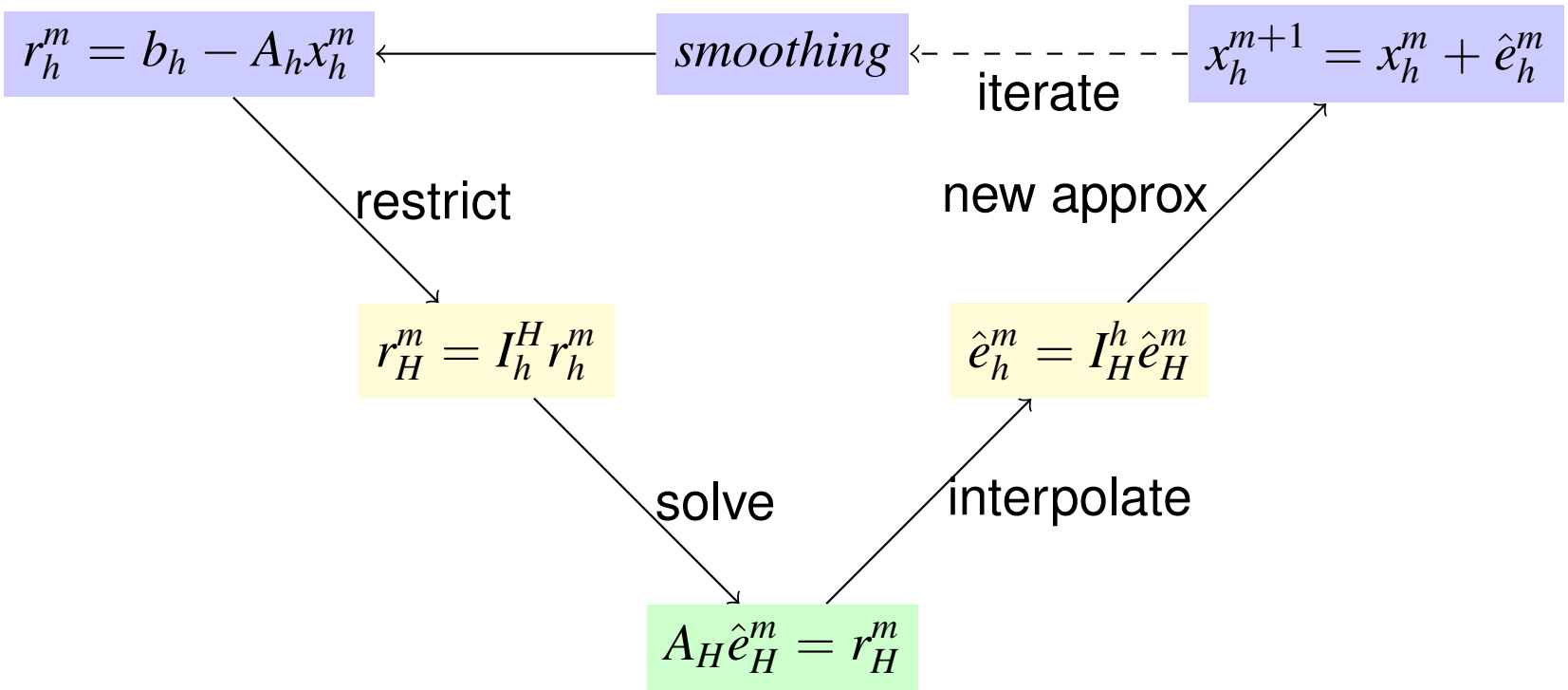
The Two-Grid: Smoothed Coarse Grid Correction

The discretized system is solved by a Two-Grid:

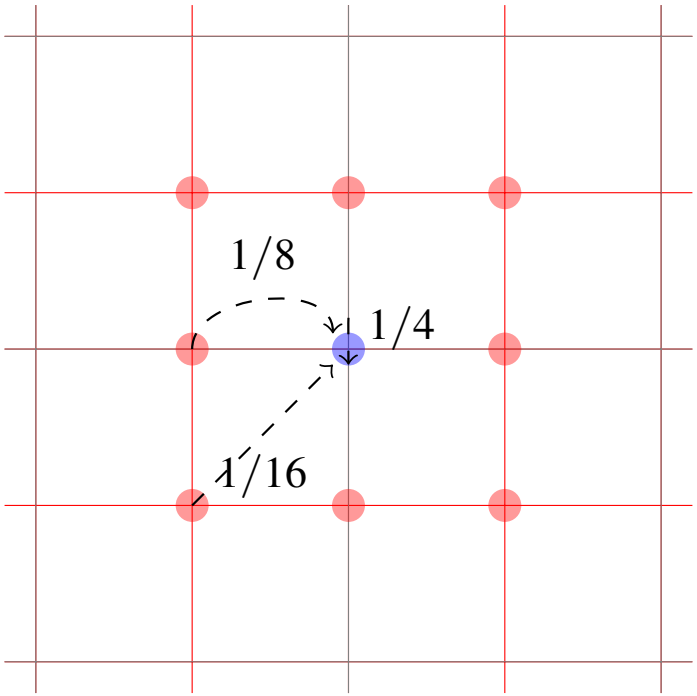
$$A\mathbf{x} = \mathbf{b}$$

$$e_h^m = x_h - x_h^m,\ r_h^m = b_h - A_h x_h^m$$

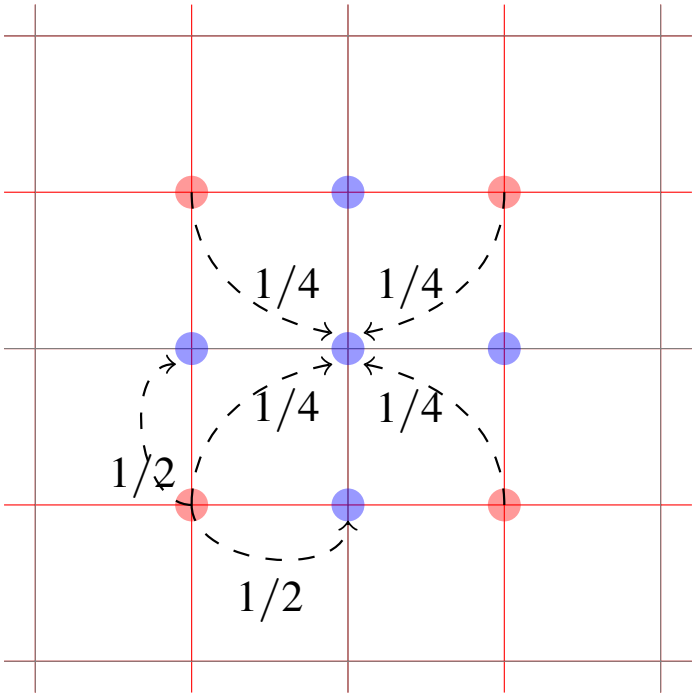
$$r_h^m = A_h e_h^m$$



restriction

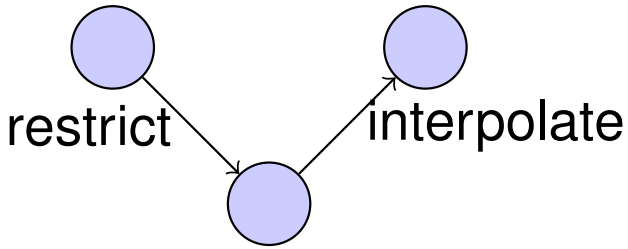


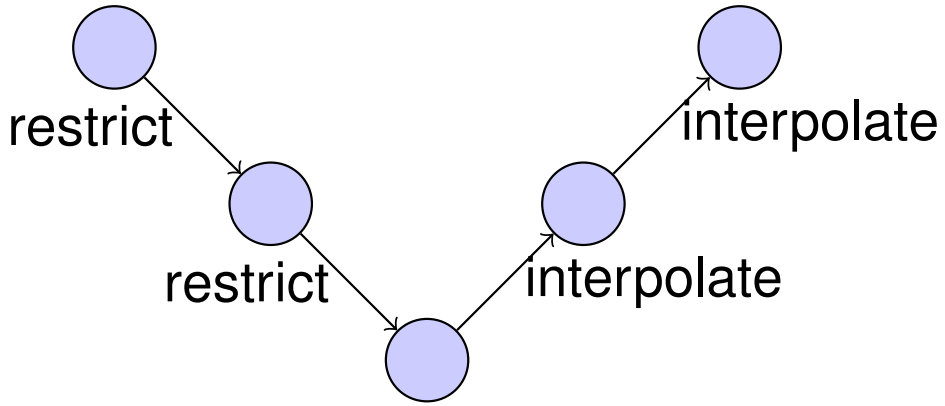
bilinear interpolation



Multigrid

from Two-Grid to Multigrid





Depending on how the recursion is coded, some variants of the V-cycle can be produced.

- grid-independence convergence
- iterative solver: reuse information
- $\mathcal{O}(n)$ algorithm

Anisotropy is handled in the discretized problem