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Towards Automated Algebraic Multigrid Preconditioner Design Using Genetic Programming for Large-Scale Laser Beam Welding Simulations

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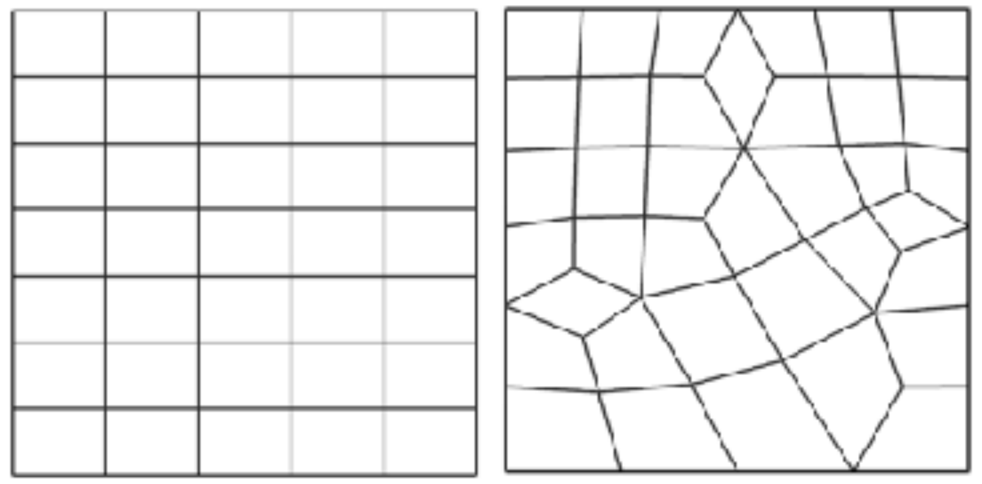
3. Center for Data and Simulation Science

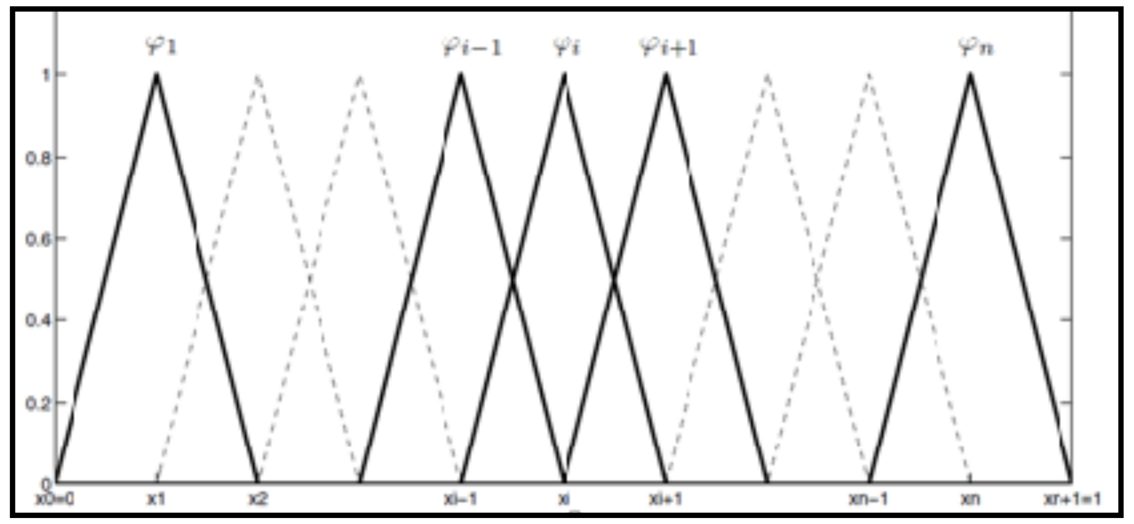
Solving Partial Differential Equations

CLASSICAL PDE SOLVERS

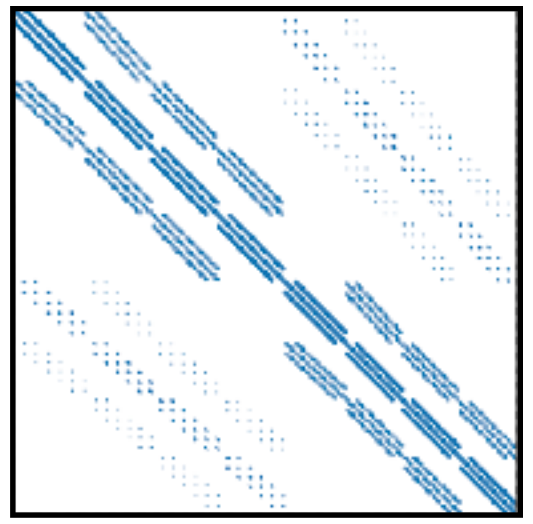
1. Generate a mesh



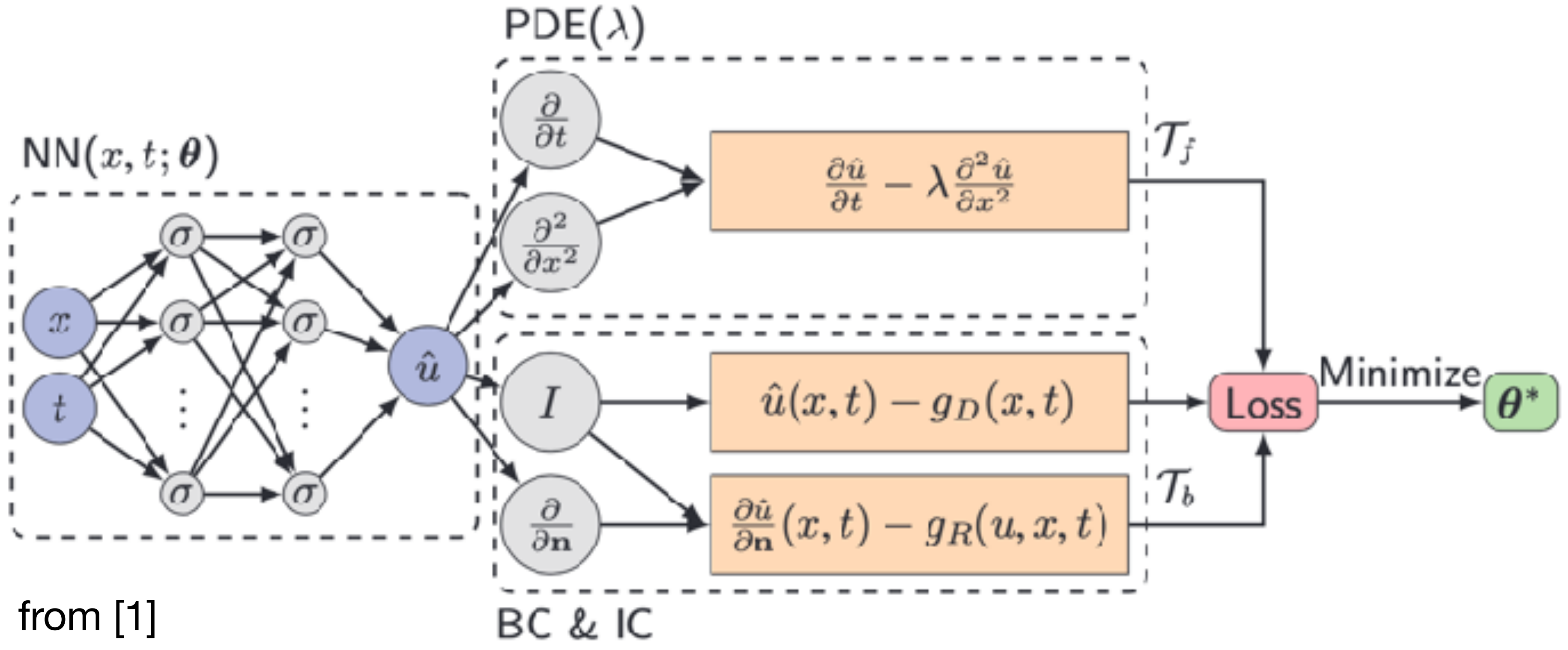
2. Apply discretization scheme



3. Solve the algebraic system



NEURAL PDE SOLVERS



from [1]

Promising conceptually[1]

- Meshless methods
- Basis functions are implicitly learnt
- Requires no specialised algebraic solvers

Reality is different

- Loss landscape is ill-conditioned[2]
- Suffers from spectral bias[3]
- Do not outperform classical methods[4]

[1] Lu, L., Meng, X., Mao, Z. and Karniadakis, G.E. 2021. **DeepXDE: A Deep Learning Library for Solving Differential Equations.** *SIAM Review*. 63, 1 (2021), 208–228. DOI:https://doi.org/10.1137/19m1274067.
[2] Chuang, P.-Y. and Barba, L. 2022. **Experience report of physics-informed neural networks in fluid simulations: pitfalls and frustration.** *Proceedings of the 21st Python in Science Conference*. (2022), 28–36. DOI:https://doi.org/10.25080/majora-212e5952-005.
[3] Cao, Y., Fang, Z., Wu, Y., Zhou, D.-X. and Gu, Q. 2021. **Towards Understanding the Spectral Bias of Deep Learning**. *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence*. (2021), 2205–2211. DOI:https://doi.org/10.24963/ijcai.2021/304.
[4] Grossmann, T.G., Komorowska, U.J., Latz, J. and Schönlieb, C.-B. 2024. **Can physics-informed neural networks beat the finite element method?** *IMA Journal of Applied Mathematics*. 89, 1 (2024), 143–174. DOI:https://doi.org/10.1093/imamat/hxae011.

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Rethinking The Role of AI

High-level Domain-Specific Languages

pystencils — speed up stencil computations on numpy arrays

Firedrake

FEniCS Project

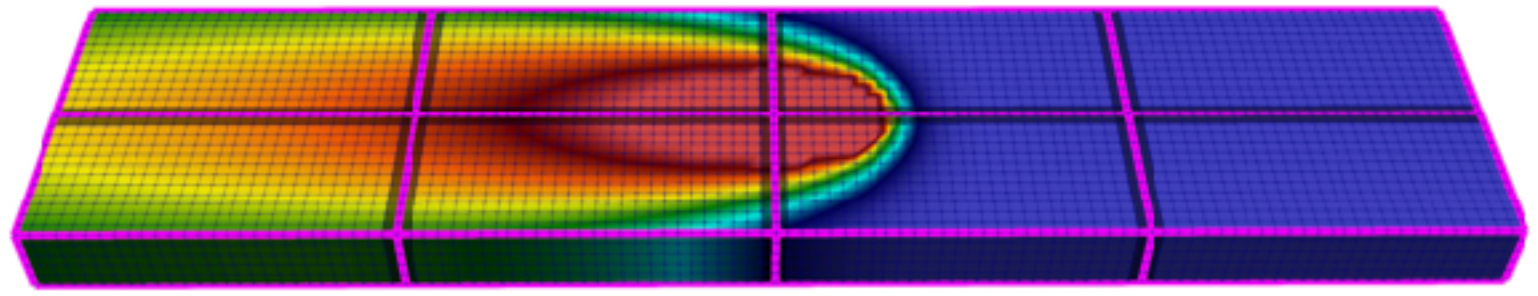
High-Performance Solver Libraries

hypre

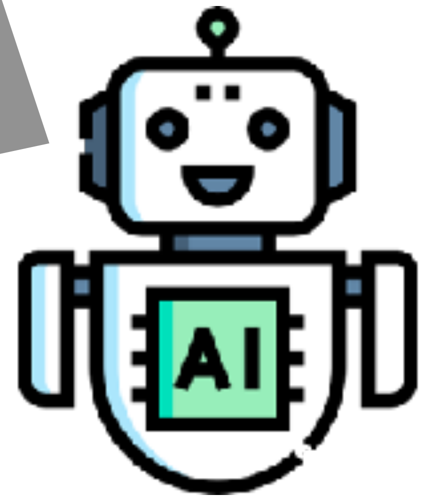
TRILINOS

PETSc

Generate efficient low-level solver code



AI for automated algorithm design



- ✓ Built upon well-tested infrastructures
- ✓ Reliable and grounded in physics
- ✓ Lowers barrier to entry for non-experts

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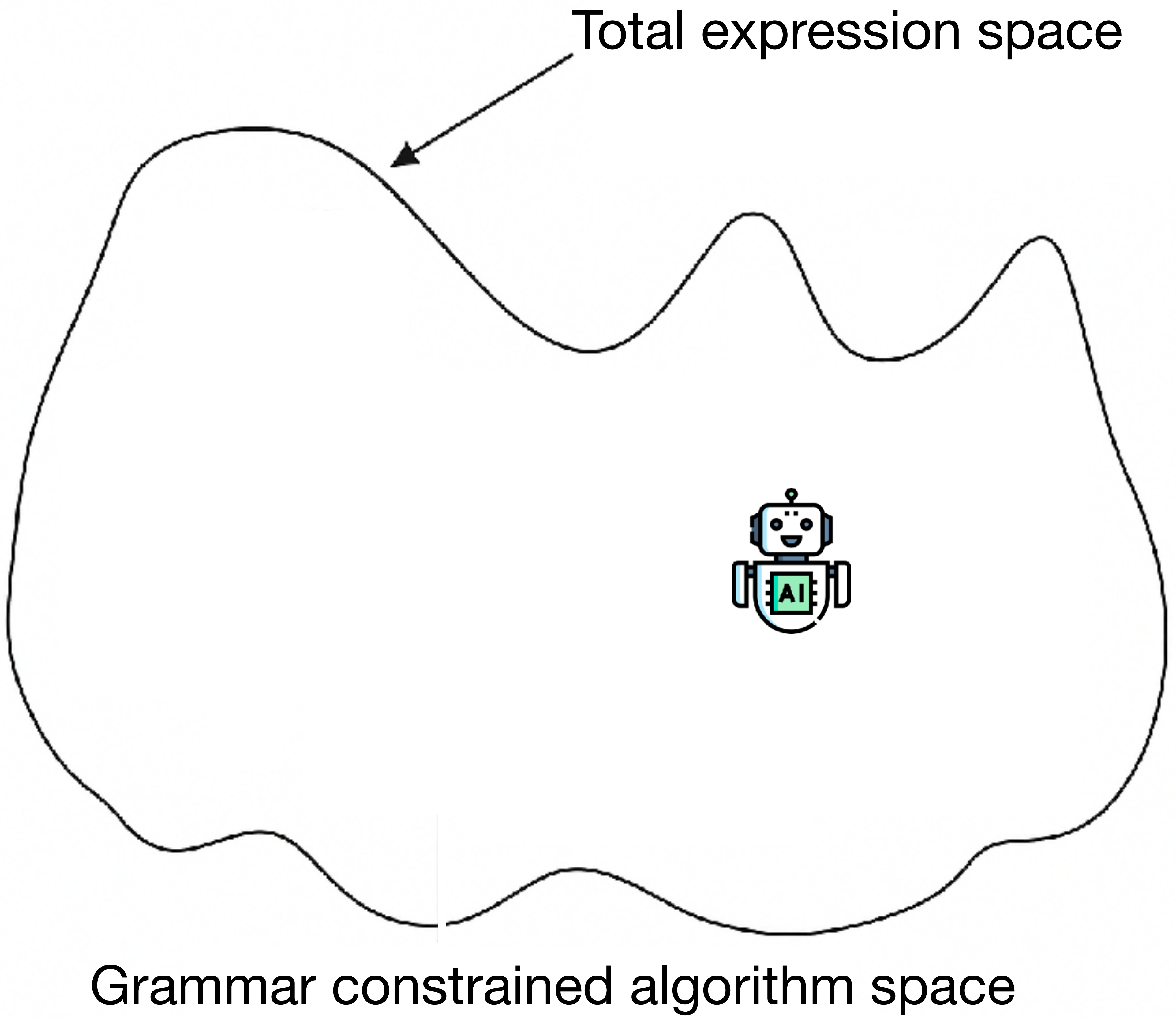
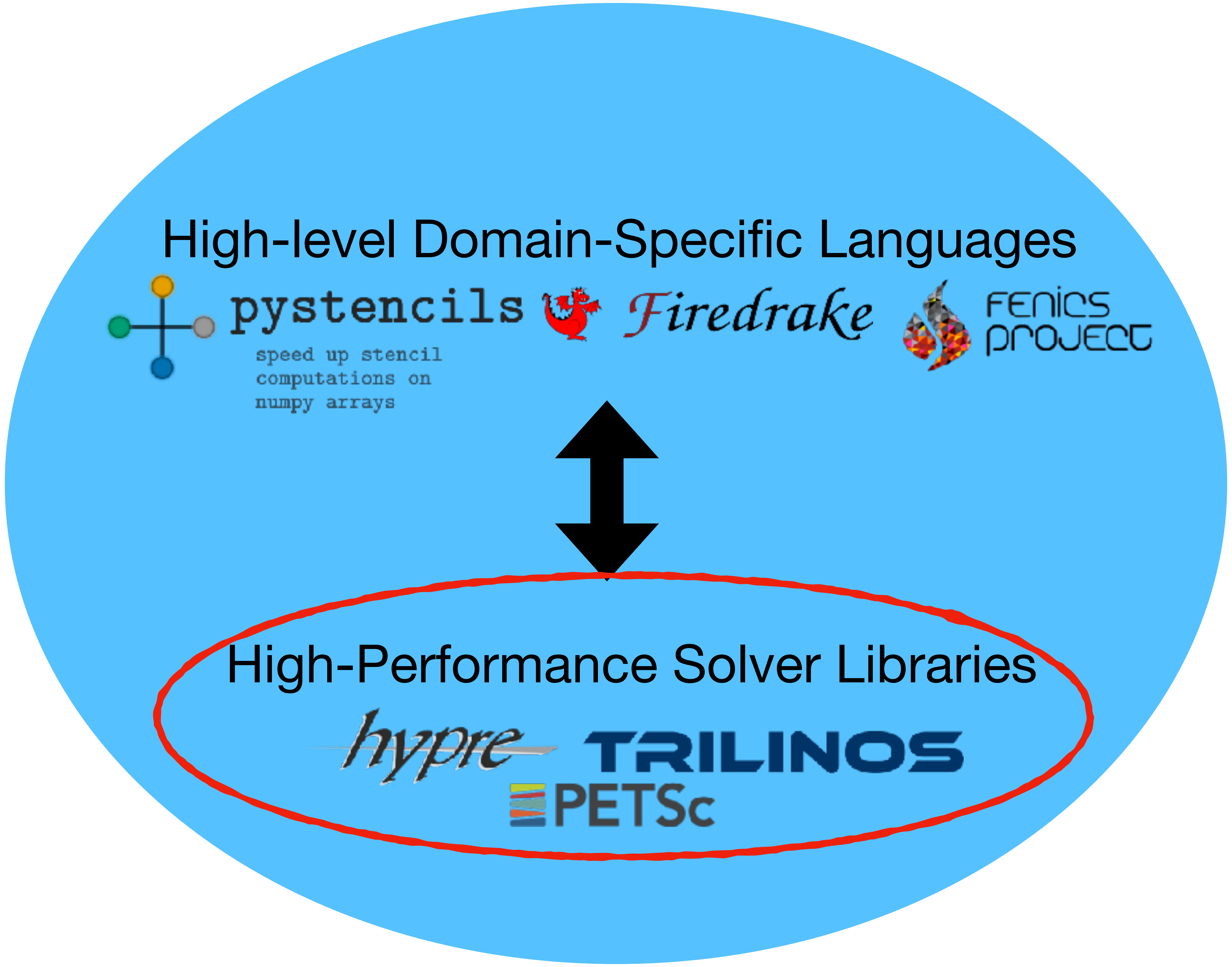
Context-Free Grammars



- ✓ Reduce search space
- ✓ Syntactically valid
- ✓ Infuse domain knowledge
- ✓ Ensure algorithmic correctness

Grammar for Multigrid Methods



$\langle S \rangle \models \langle s_f \rangle$	$\langle M_{l_1} \rangle \models l_1$ *GS Fwd./Bwd.*
$\langle s_f \rangle \models l_1\text{RELAX}(\langle M_{l_1} \rangle, \langle \mathcal{R} \rangle, \langle s_f \rangle)$	l_1 *Jacobi*
$\text{HYBRIDRELAX}(\langle M_H \rangle, \langle w_i \rangle, \langle w_o \rangle, \langle \mathcal{R} \rangle, \langle s_f \rangle)$	$\langle M_H \rangle \models$ *GS Fwd.*
$\text{JACOBIRELAX}(\langle M_J \rangle, \langle w \rangle, \langle \mathcal{R} \rangle, \langle s_f \rangle)$	*GS Bwd.*
$\text{COARSEGRIDCORRECTION}(\langle \alpha \rangle, \langle s_{f-1} \rangle)$	$\langle M_J \rangle \models$ *Jacobi*
INITIALGUESS	$\langle \mathcal{R} \rangle \models$ *Lexicographic*
$\langle s_c \rangle \models \text{RESTRICTANDSOLVE}(A_c^{-1}, \langle s_{c+1} \rangle)$	*CF-relaxation*
$\langle s_k \rangle \models l_1\text{RELAX}(\langle M_{l_1} \rangle, \langle \mathcal{R} \rangle, \langle s_k \rangle)$	$\langle w_i \rangle \models \omega_1 \mid \omega_2 \mid \ldots \mid \omega_m$
$\text{HYBRIDRELAX}(\langle M_H \rangle, \langle w_i \rangle, \langle w_o \rangle, \langle \mathcal{R} \rangle, \langle s_k \rangle)$	$\langle w_o \rangle \models \beta_1 \mid \beta_2 \mid \ldots \mid \beta_n$
$\text{JACOBIRELAX}(\langle M_J \rangle, \langle w \rangle, \langle \mathcal{R} \rangle, \langle s_k \rangle)$	$\langle w \rangle \models \delta_1 \mid \delta_2 \mid \ldots \mid \delta_p$
$\text{RESTRICT}(\langle s_{k+1} \rangle)$	$\langle \alpha \rangle \models \gamma_1 \mid \gamma_2 \mid \ldots \mid \gamma_r$
$\text{COARSEGRIDCORRECTION}(\langle \alpha \rangle, \langle s_{k-1} \rangle)$	

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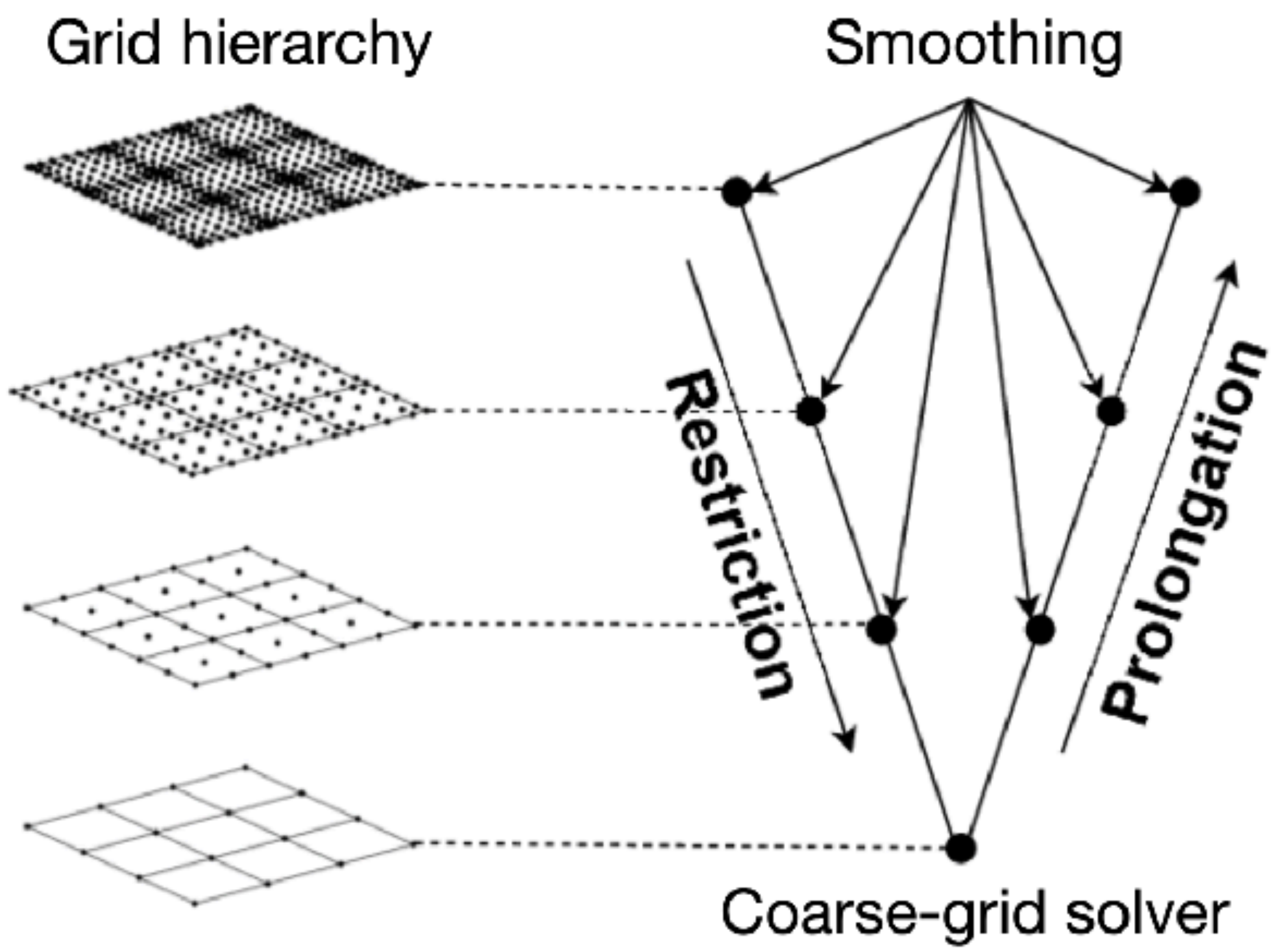
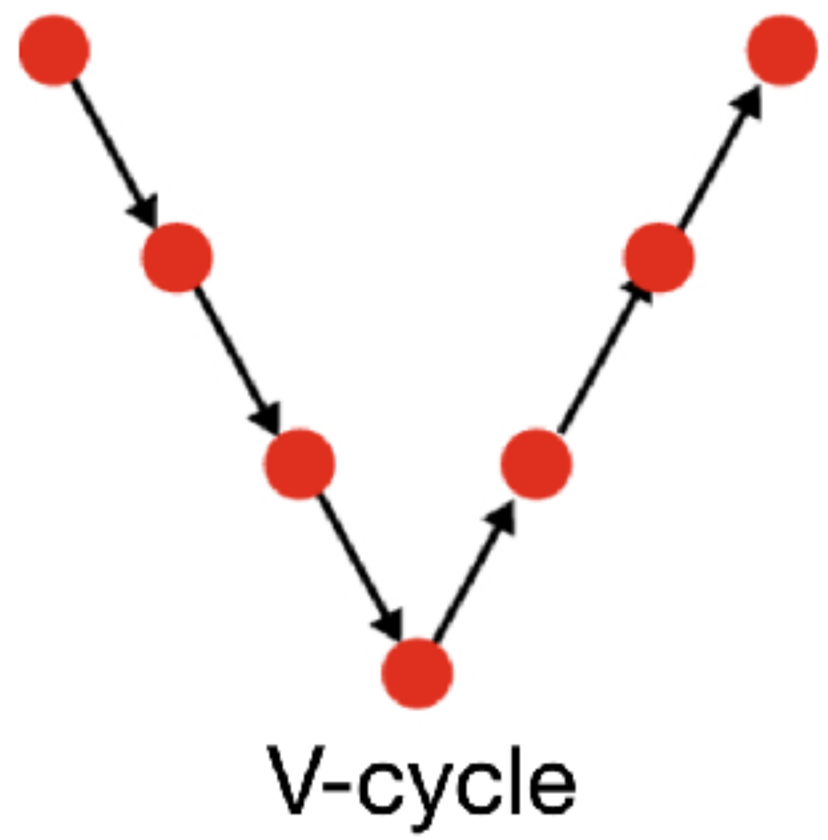
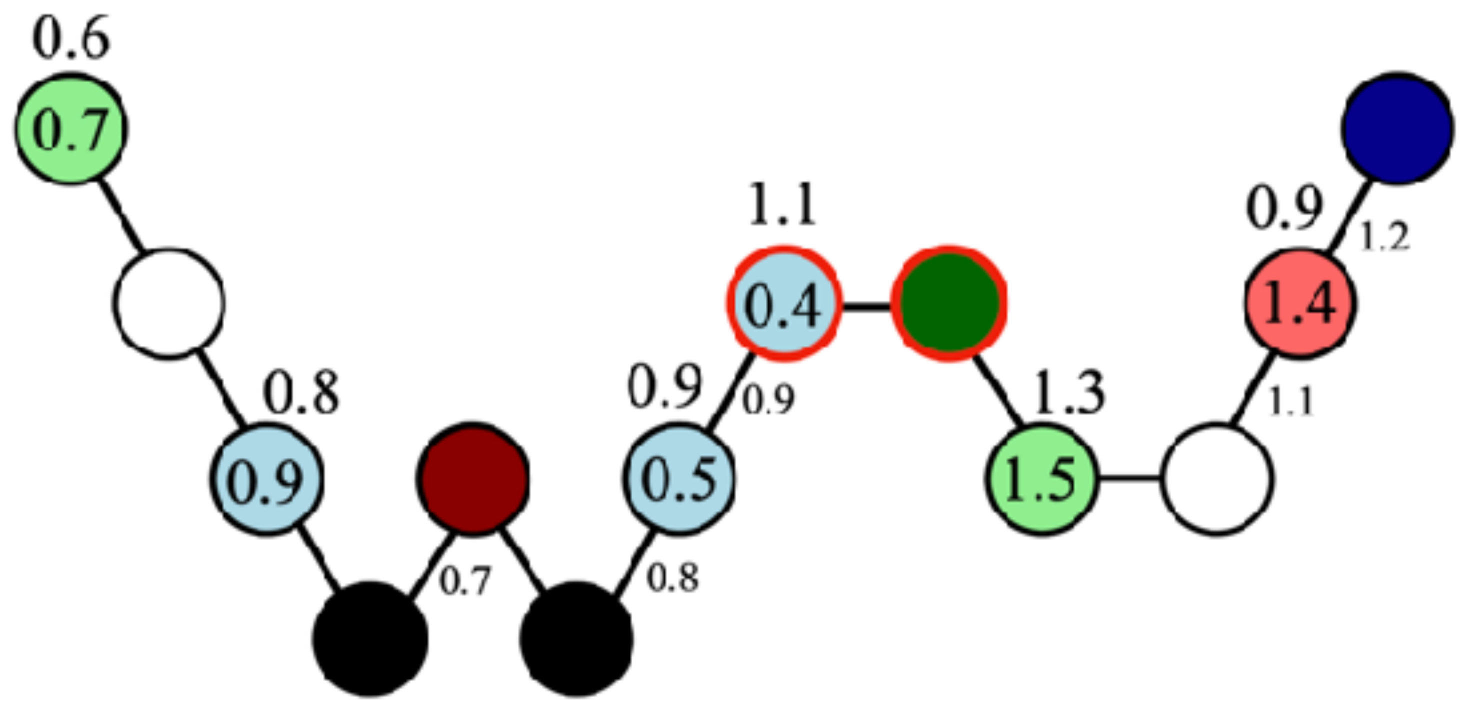
Multigrid Methods







Requires less than **30 FLOPS per unknown** to solve a 2D Poisson to **discretization accuracy**![5]

★ **Need to navigate a large search space**

★ **A well-designed multigrid method is very hard to beat**

[5] Stüben, K., & Trottenberg, U. **Multigrid methods: Fundamental algorithms, model problem analysis and applications,** in vol. 960 of Lecture Notes in Mathematics. Springer Verlag, 1982

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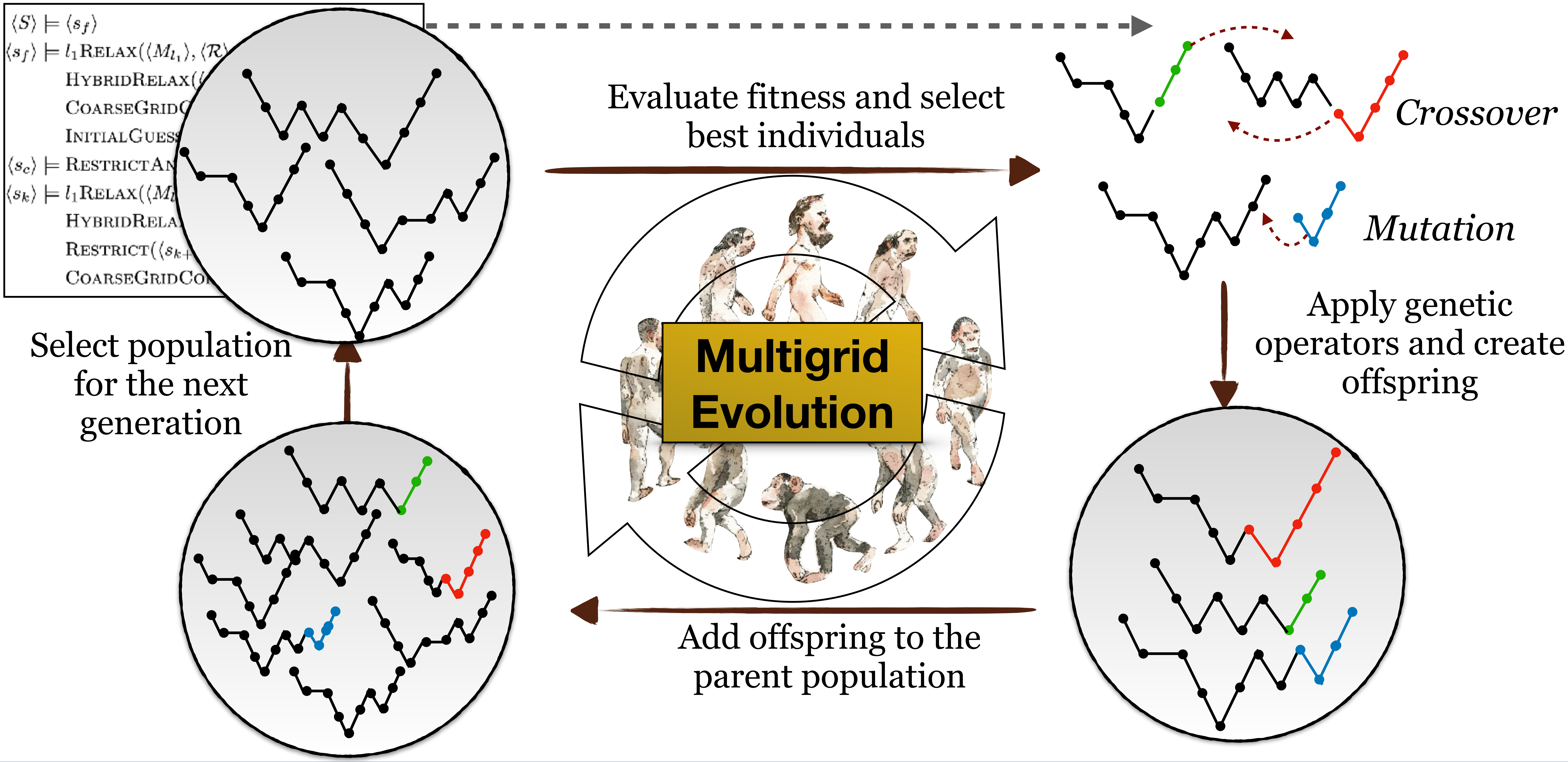
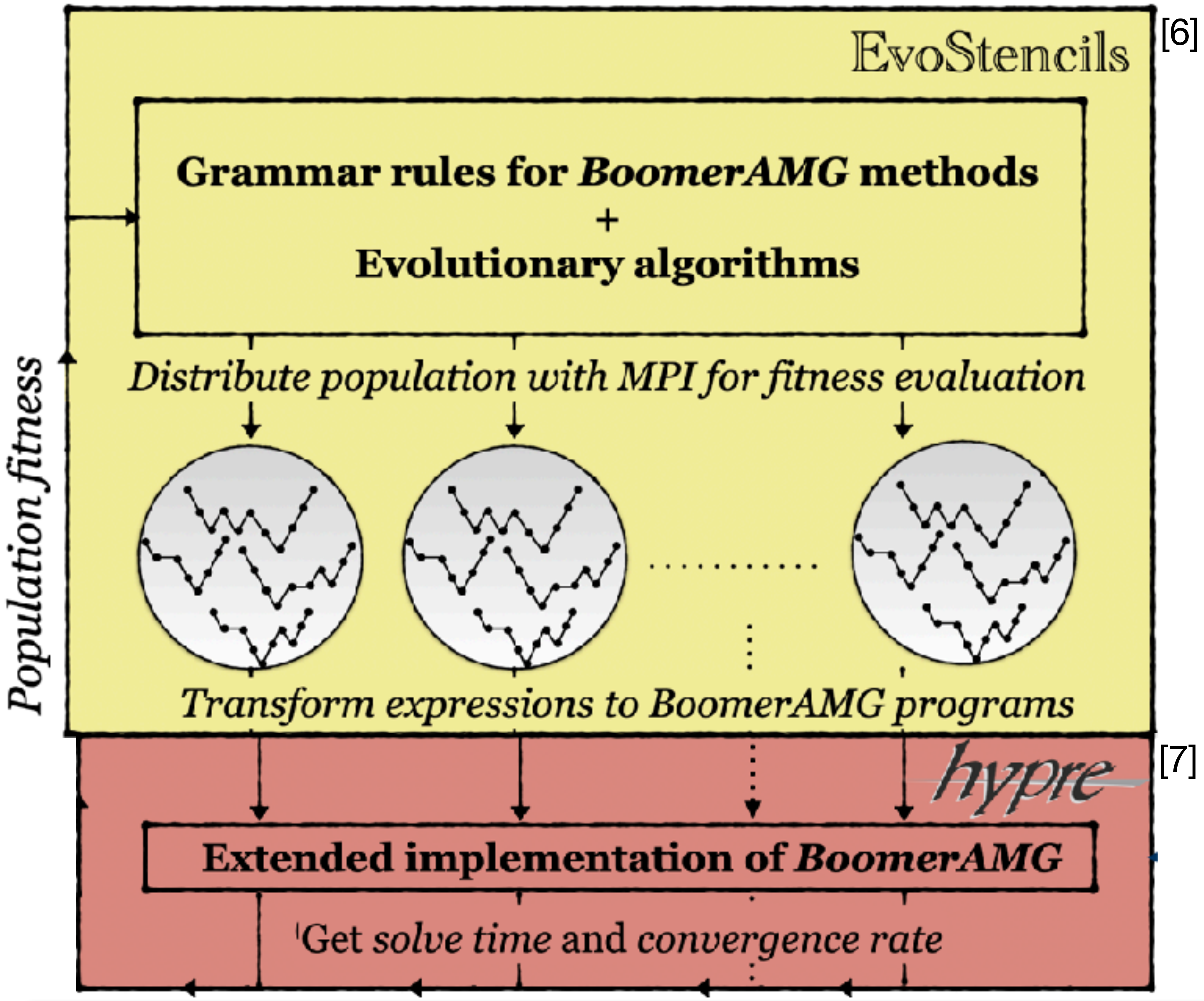
Grammar-Guided Genetic Programming For Multigrid



Software

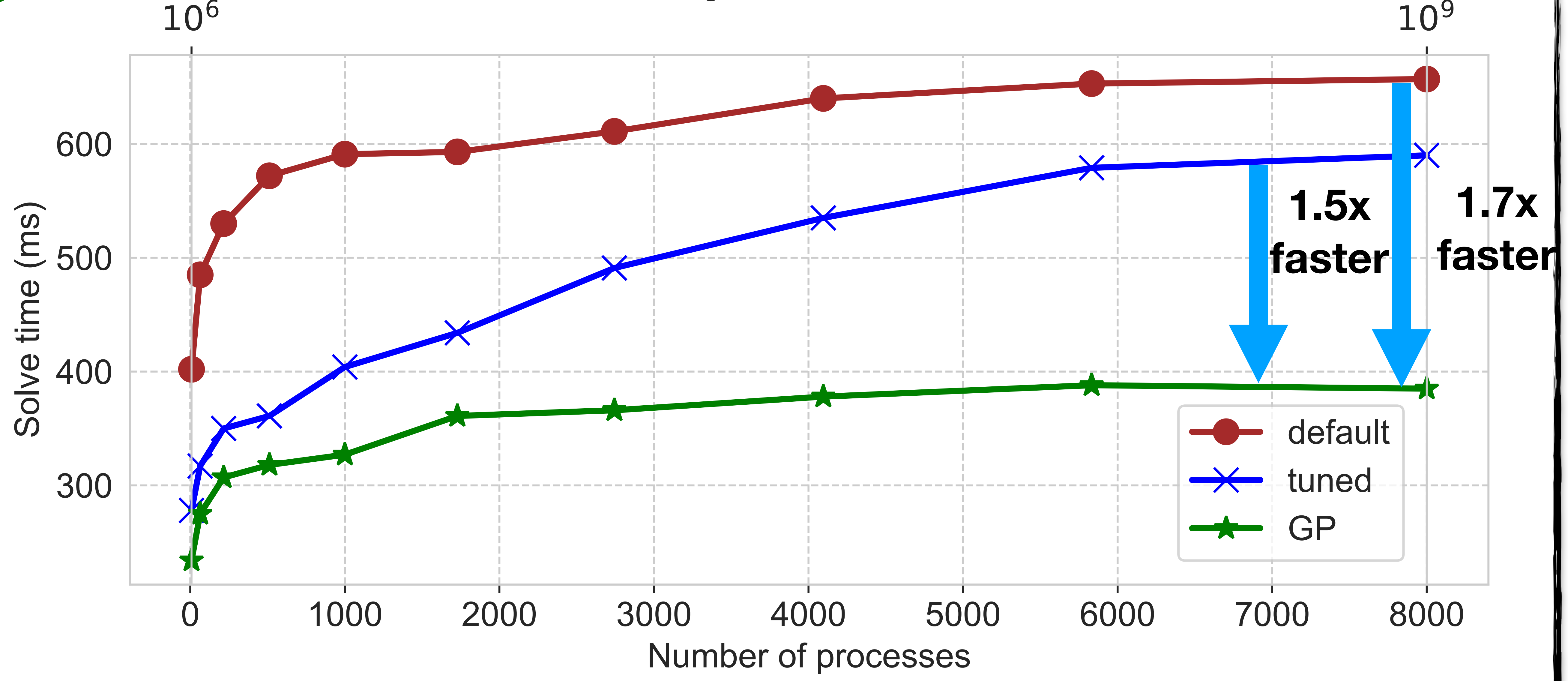


[6] Schmitt, J., Kuckuk, S. & Köstler, H. **EvoStencils: a grammar-based genetic programming approach for constructing efficient geometric multigrid methods.** Genet Program Evolvable Mach 22, 511–537 (2021). https://doi.org/10.1007/s10710-021-09412-w

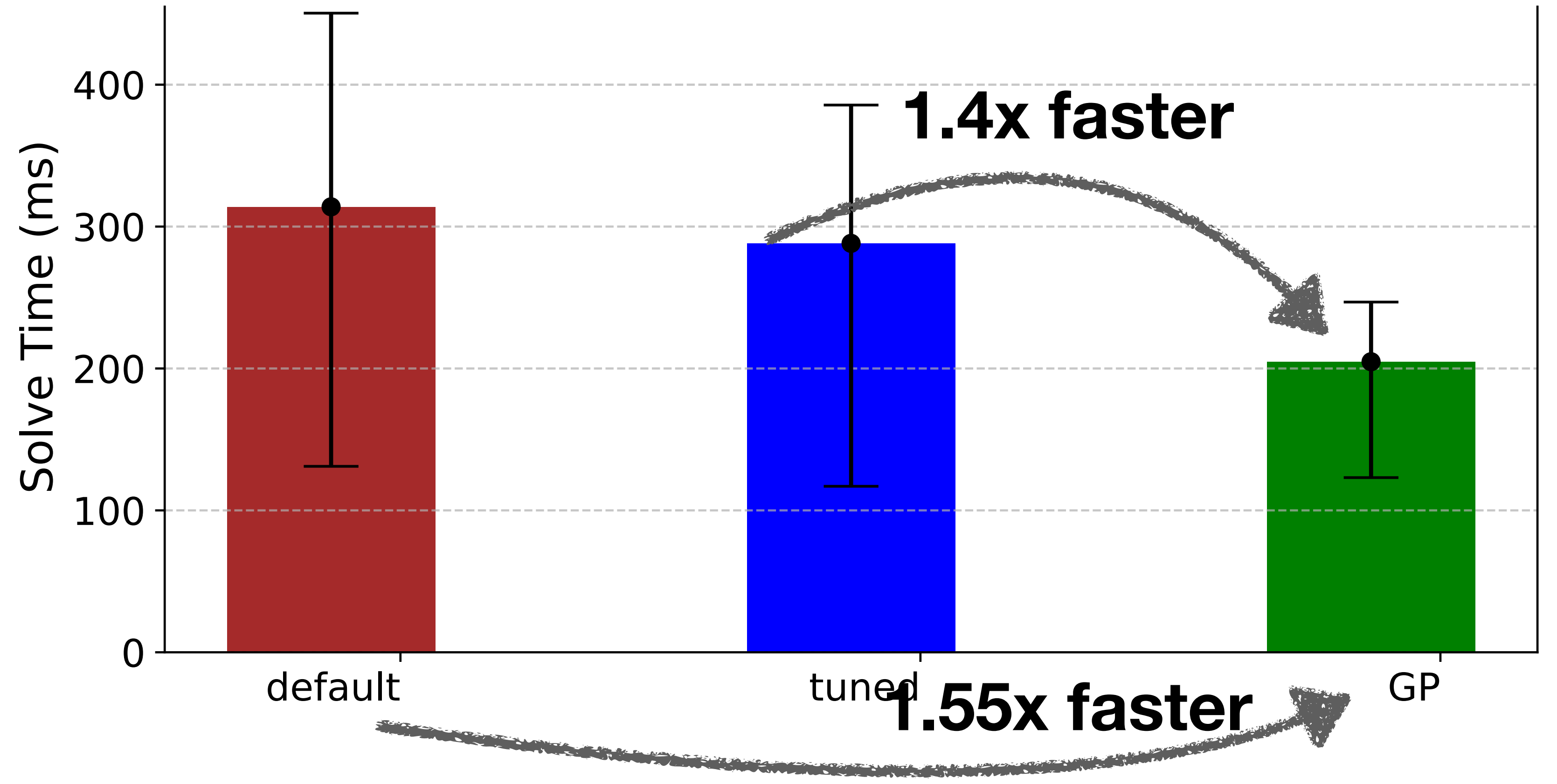
[7] Parthasarathy, D., Mitchell, W.B., Köstler, H. (2024). **Evolving Algebraic Multigrid Methods Using Grammar-Guided Genetic Programming**. arXiv preprint arXiv:2412.05852.

The lower, the better

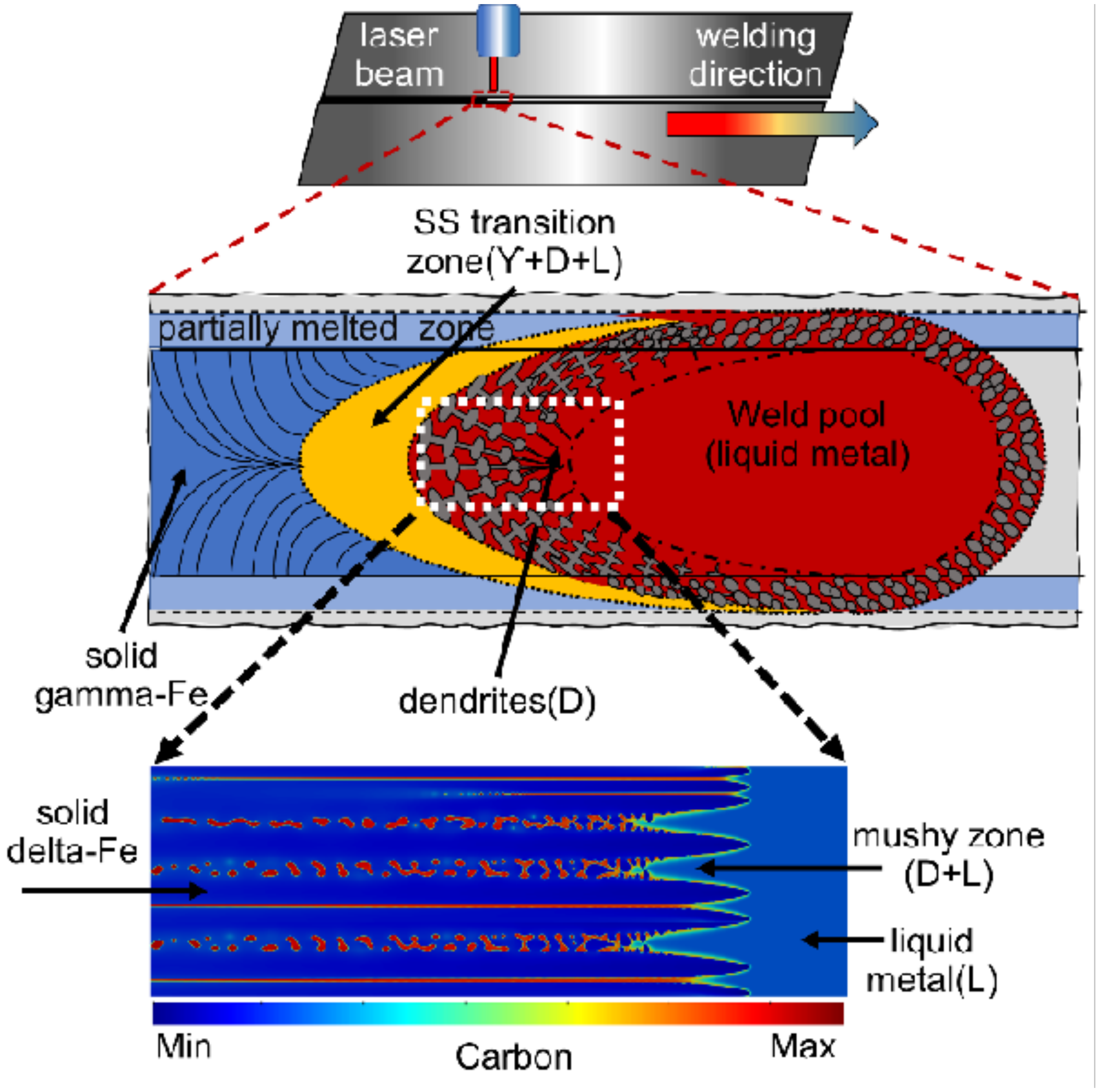
I. Stationary 3D anisotropic diffusion



II. Time-stepping multiphysics ICF simulations



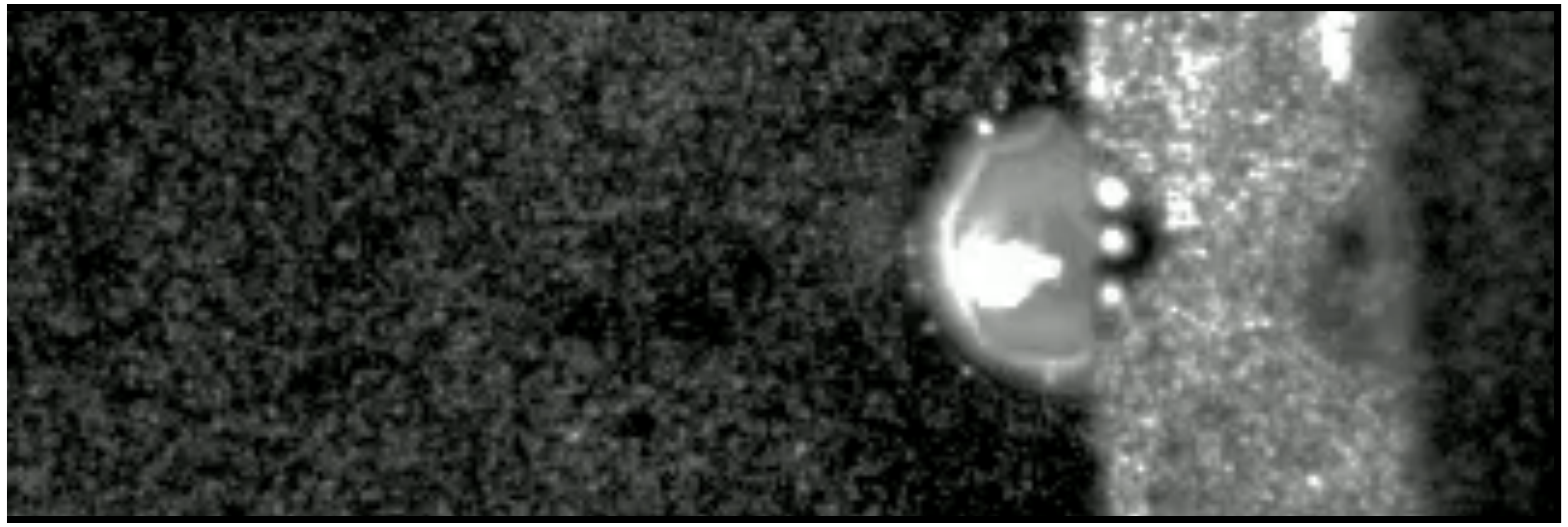
Laser Beam Welding



DFG research group 5134

"Solidification Cracks During Laser Beam Welding – High Performance Computing for High Performance Processing"

https://www.for5134.science/en



Thermo-Mechanical Simulation

1. Continuous formulation
Thermoelasticity equations

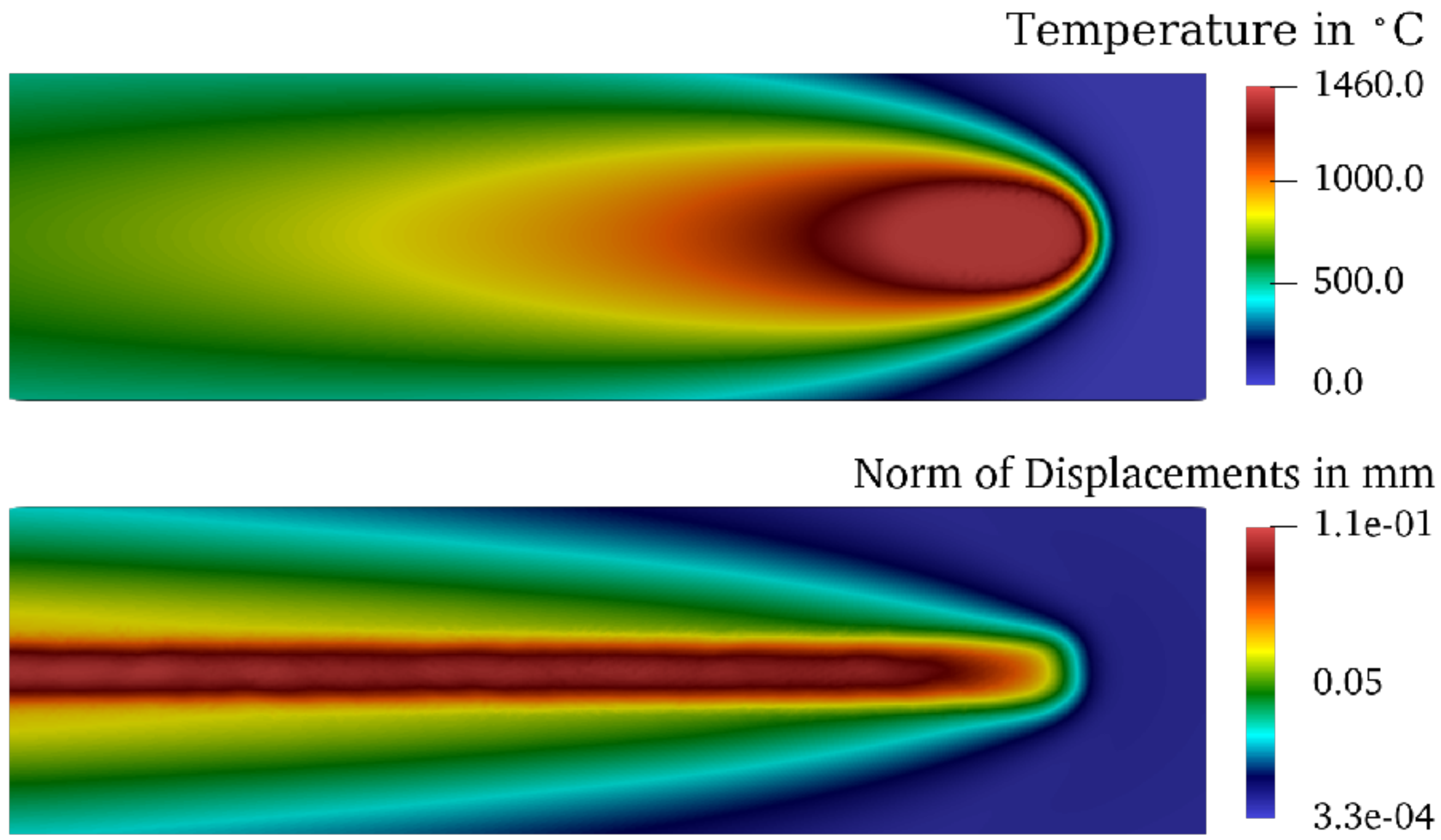
$$\mathrm{div}(\sigma(u,\theta)) + \rho \mathbf{b} = 0$$
$$\mathrm{div}(\mathbf{q}) + \gamma\, \mathrm{div}(\dot{u})\theta + \rho\, c_\rho \dot{\theta} = \rho r$$

2. Discretization and linearisation
Saddle point system

$$K\Delta\mathbf{d} = \begin{bmatrix} K_{uu} & K_{u\theta} \\ K_{\theta u} & K_{\theta\theta} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{d}_u \\ \Delta\mathbf{d}_\theta \end{bmatrix} = \begin{bmatrix} R_u \\ R_\theta \end{bmatrix} = R$$

3. Solve Ax = b
AMG preconditioned solvers

hypre



Thermo-mechanical simulation of the welding plate[8]

[8] Bevilacqua, T., Gumenyuk, A., Habibi, N., Hartwig, P., Klawonn, A., Lanser, M., Rethmeier, M., Scheunemann, L., Schröder, J. (2025). **Large-scale Thermo-Mechanical Simulation of Laser Beam Welding Using High-Performance Computing: A Qualitative Reproduction of Experimental Results.** arXiv preprint arXiv:2503.09345.

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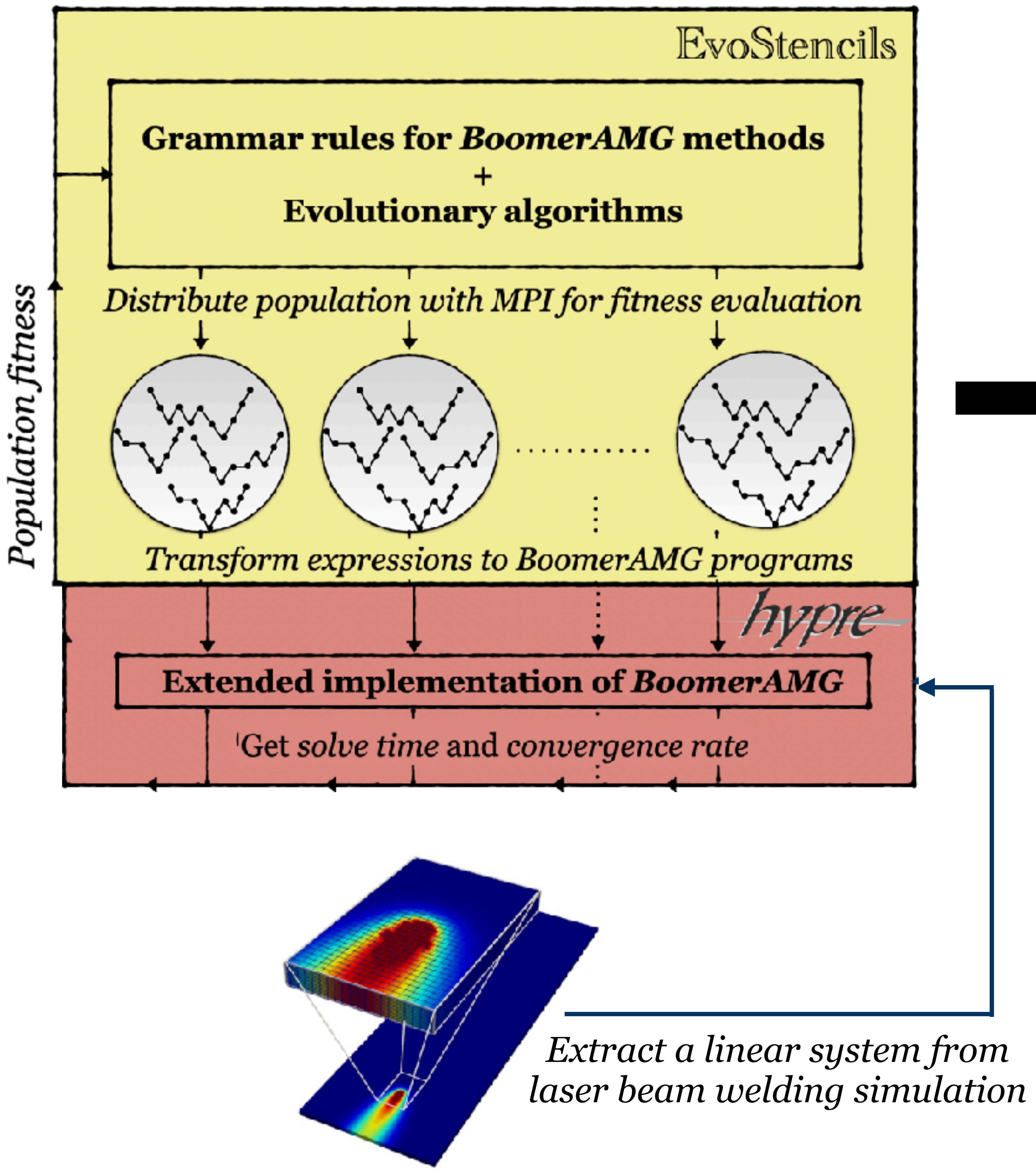
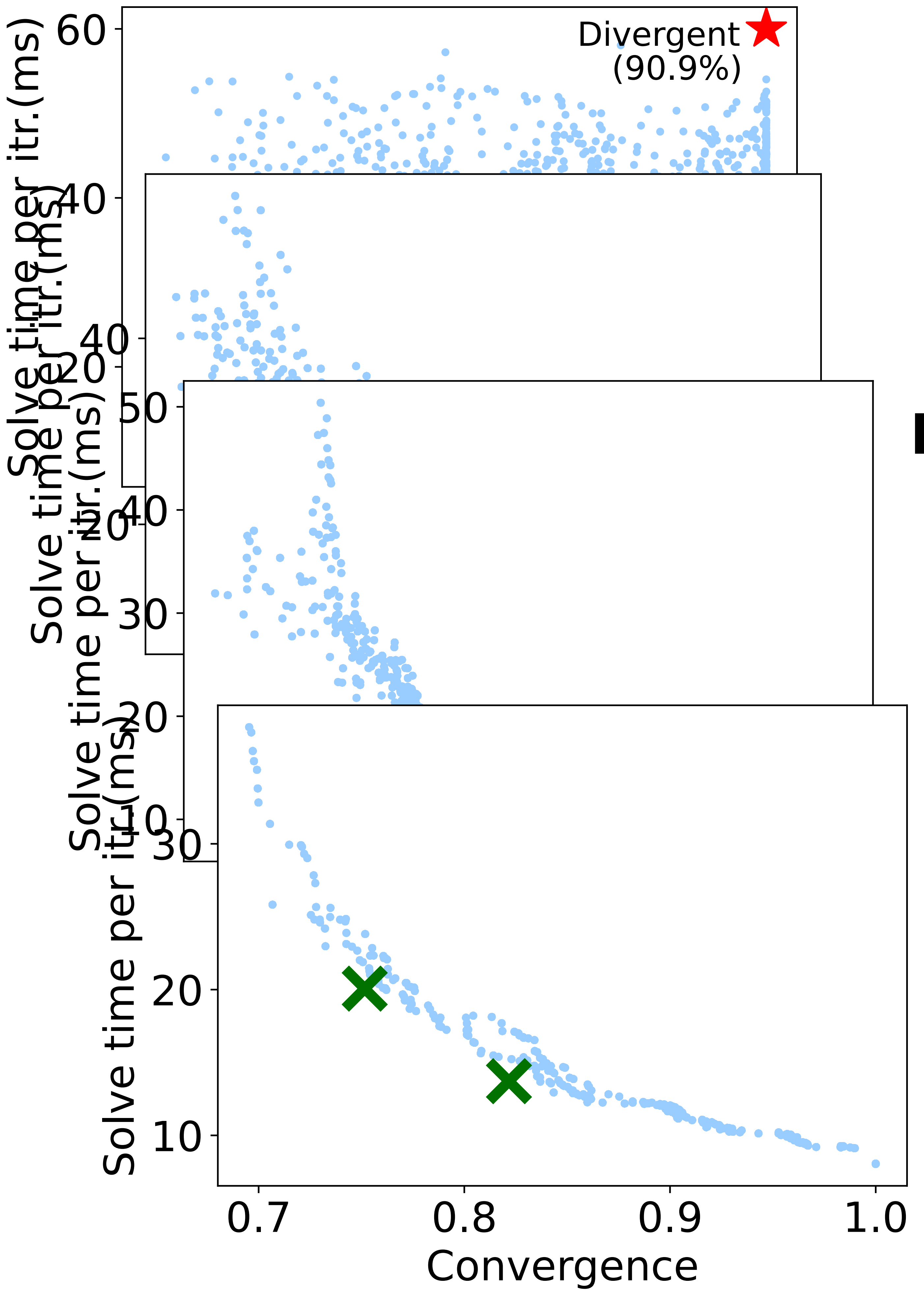
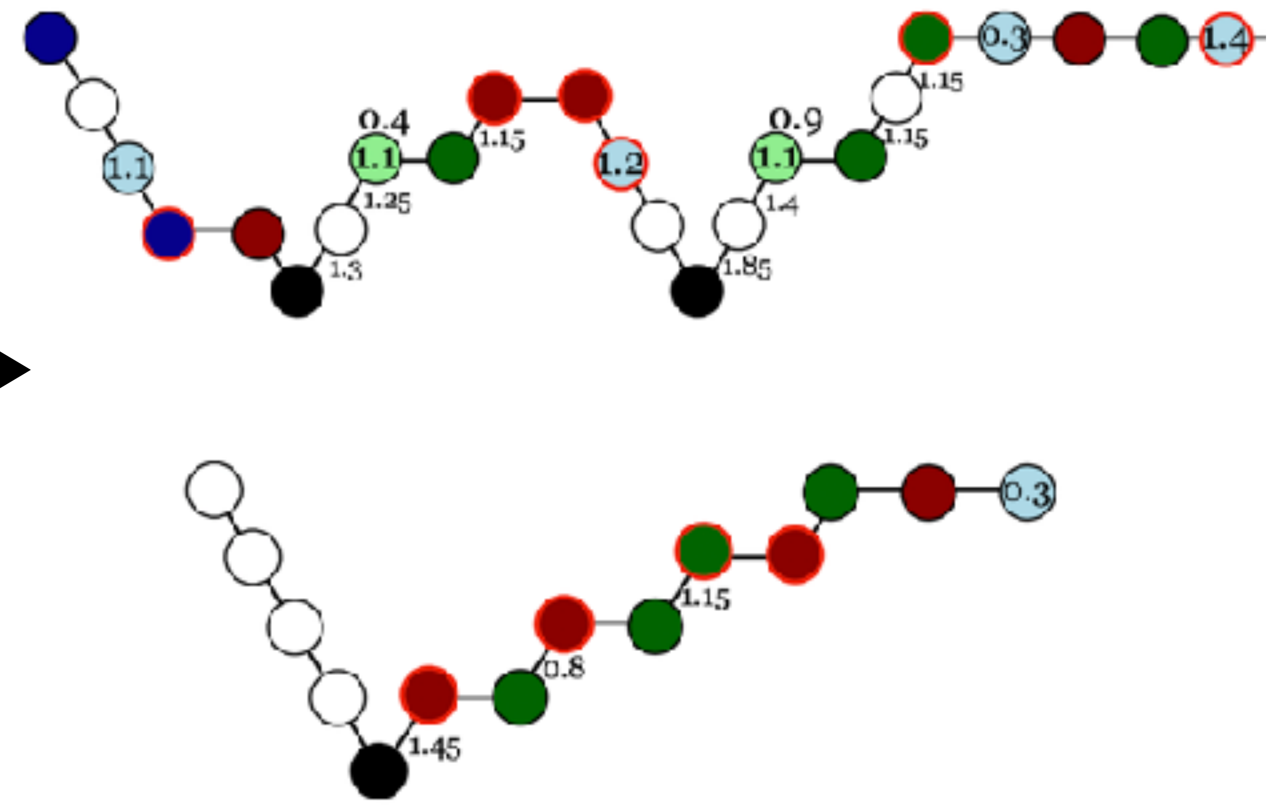
Automated AMG Design







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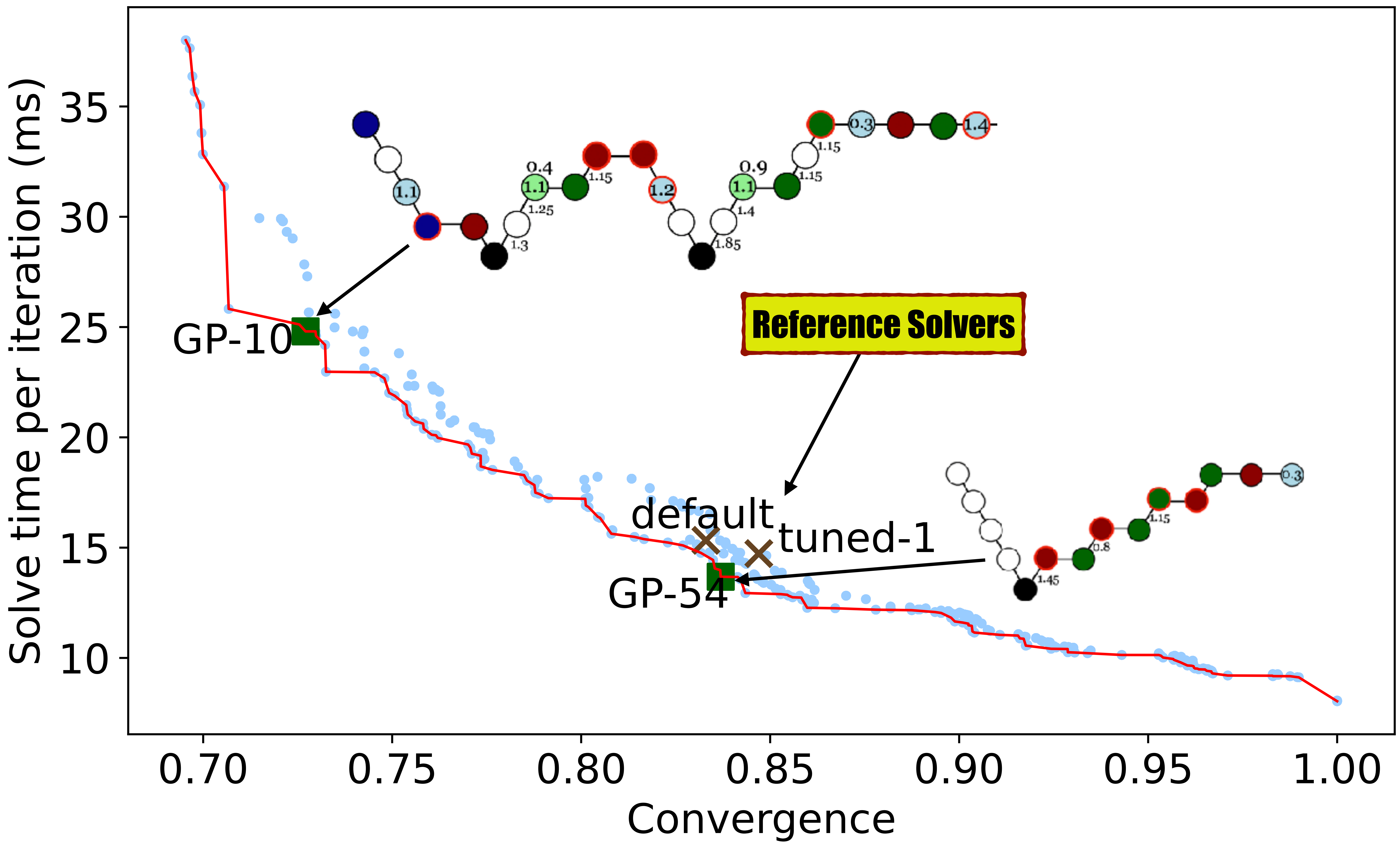
Final Population of Solvers



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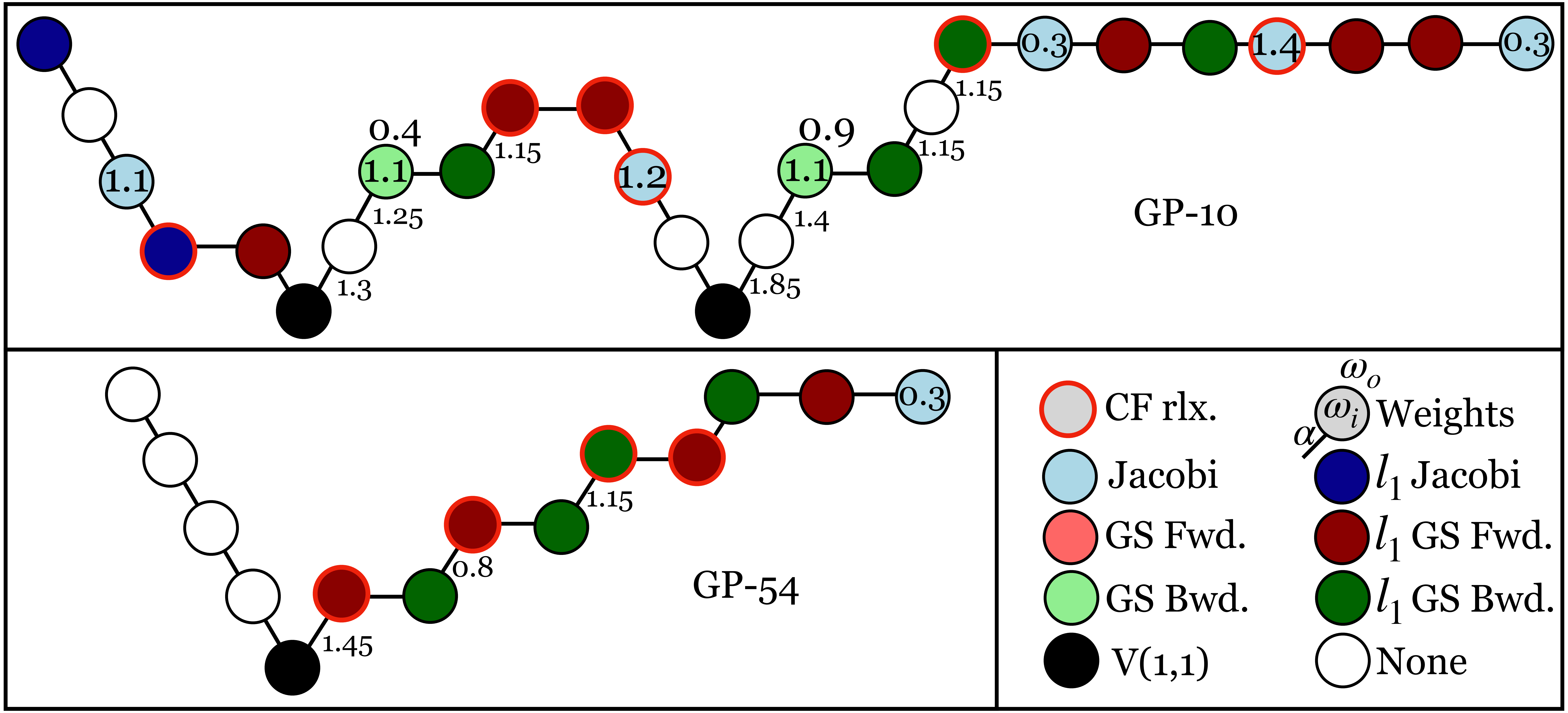
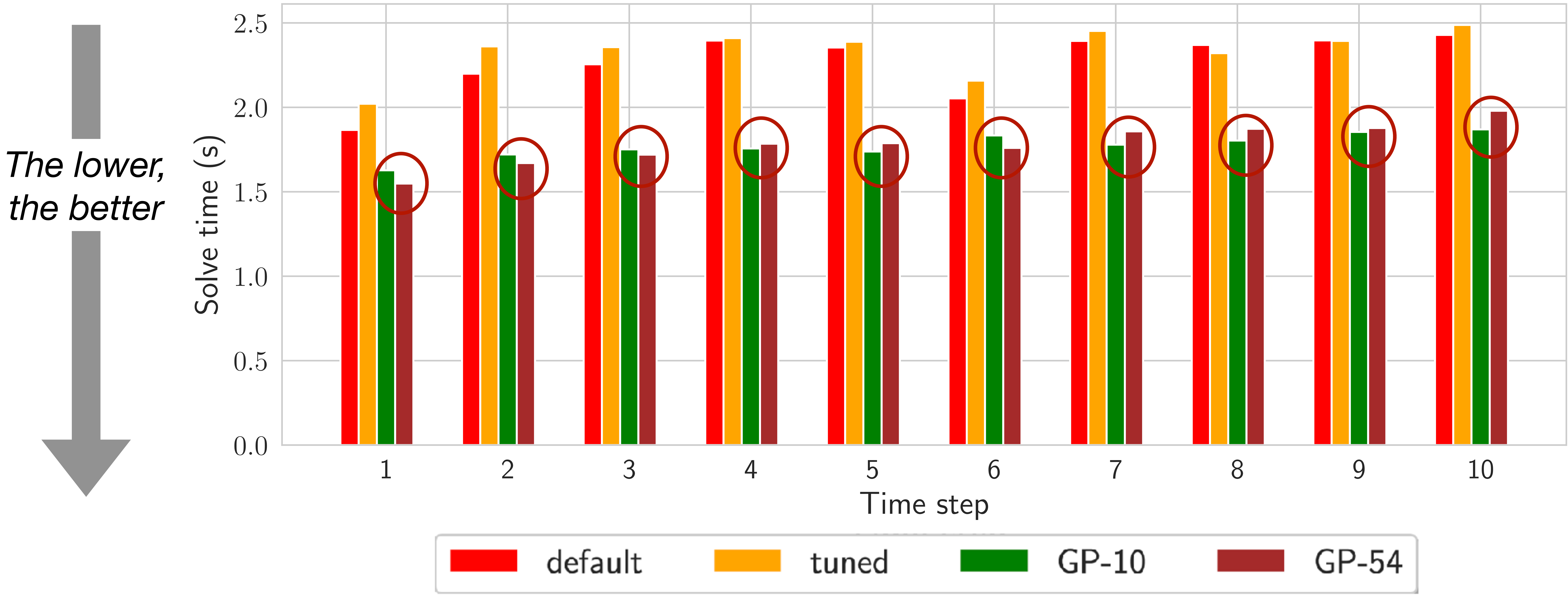
Flexible GP-AMG Methods

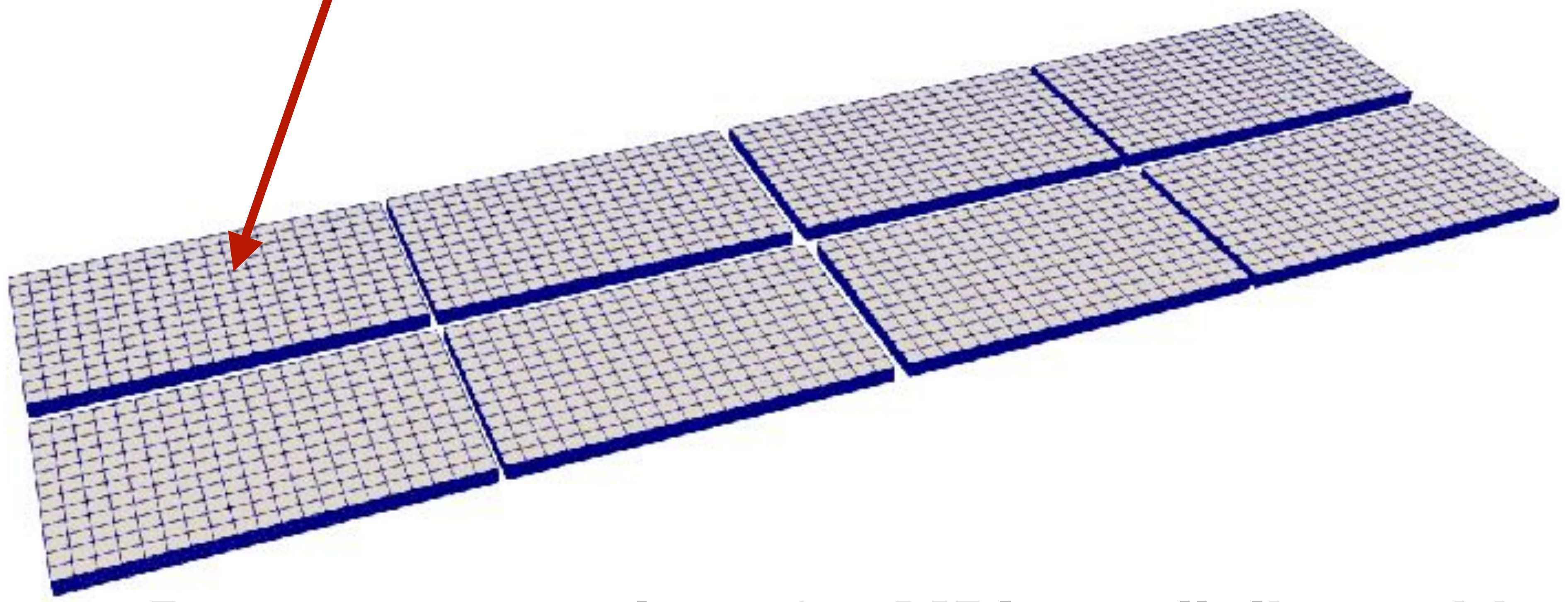


Solve Time for 89,000 DOFs



Scalability

1 MPI process per tile



Processor topology for MPI parallelism with 89,000 DOFs

	GP-10		GP-22		GP-54	
DOFs	T(s)	N	T(s)	N	T(s)	N
89 100	17.7	89	**17.1**	101	17.9	162
347 116	24.7	117	**22.8**	125	24.3	206
1 370 028	**277.6**	984	279.1	1155	326.8	2003

	default		tuned-1		speedup	
DOFs	T(s)	N	T(s)	N	η_1	η_2
89 100	22.7	149	23.3	168	1.33	1.37
347 116	31.9	188	30.9	210	1.40	1.36
1 370 028	436.7	1942	341.7	1665	1.57	1.23

Conclusion

- Grammar-guided GP discovers novel multigrid methods with superior efficiency
- Generalizes well in a time-stepping code
- Scalability could be better
- Future Work:
  - Extend the grammar to handle blocked systems
  - Evaluate the fitness over multiple proxies

TAKE-HOME MESSAGE

Automated, grammar-guided algorithm design shows encouraging results — holds great potential to address complex and challenging computational problems

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Thanks for listening!

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arXiv preprint

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