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Domain Decomposition Methods: Origins and Applications to Multiscale Modeling

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SAND-2018XXXX

Domain Decomposition

Historical and Mathematical Origins

Convergence Analysis

Multiscale Modeling: Atomistic-to-Continuum Coupling

Multi-Model Coupling: Classical Elasticity and Peridynamics

Domain Decomposition

Domain Decomposition generally means the splitting of a partial differential equation (PDE) into coupled problems on smaller domains forming a partition of the original domain, such that the solution to the partitioned problem is the same as the original unpartitioned problem.

This is commonly driven by the desire to utilize parallel computers.

Early drivers for domain decomposition methods arose from an inability to fit large computational models into memory.

Massively parallel computers make previously intractable problems possible, but come with the cost of developing algorithmic solution methods that parallelize well.

We're being pressed to find and exploit more parallelism in our algorithms. Need million- and billion-way parallelism.

Summit at ORNL is currently world's fastest computer at 200 petaflops (200,000 trillion floating point ops per second)

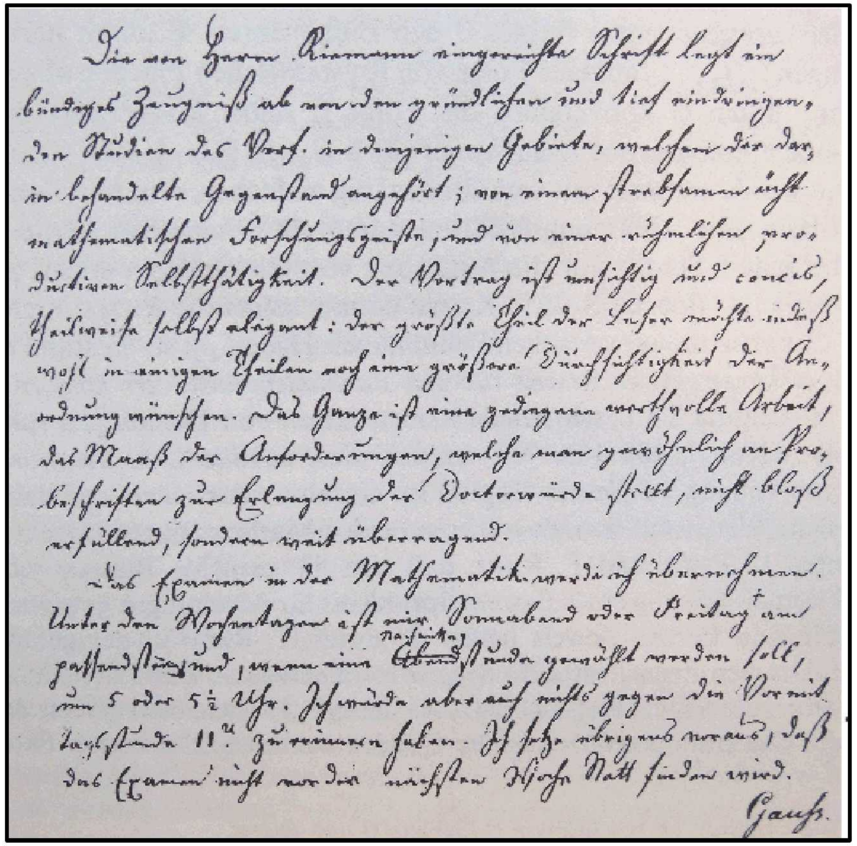
One would reasonably expect our domain decomposition story to begin with the advent of parallel computing. However, our story begins in the mid-1800s. The following historical exposition is taken from [1].

[1] Gander M, Wanner G (2013) The origins of the alternating Schwarz method. In: Erhel J, Gander M, Halpern L, Pichot G, Sassi T, Widlund O (eds) Domain decomposition methods in science and engineering XXI, Lecture Notes in Computational Science and Engineering. Springer, Berlin, pp 415–422

The Riemann Mapping Theorem

- Bernhard Riemann studied at the University of Berlin from 1847-1849.
- During his time of study, Carl Gustav Jacob Jacobi, Peter Gustav Lejeune Dirichlet, Jakob Steiner, and Gotthold Eisenstein taught there. Riemann's advisor was C.F. Gauss.
- Gauss did not praise other mathematicians easily, but wrote this about Riemann:*

Bernhard Riemann



Die von Herrn Riemann eingereichte Schrift legt ein bündiges Zeugniß ab von den gründlichen und tief eindringenden Studien des Verf. in demjenigen Gebiete, welchem der darin behandelte Gegenstand angehört; von einem strebsamen ächt mathematischen Forschungsgeiste, und von einer rühmlichen productiven Selbstthätigkeit. Der Vortrag ist umsichtig und concis, theilweise selbst elegant: der größte Theil der Leser möchte indeß wohl in einigen Theilen noch eine größere Durchsichtigkeit der Anordnung wünschen. Das Ganze ist eine gediegene werthvolle Arbeit, das Maaß der Anforderungen, welche man gewöhnlich an Probeschriften zur Erlangung der Doctorwürde stellt, nicht bloß erfüllend, sondern weit überragend.

Das Examen in der Mathematik werde ich übernehmen. Unter den Wochentagen ist mir Sonnabend oder Freitag am passendsten, und, wenn eine Nachmittagsstunde gewählt werden soll, um 5 oder 5½ Uhr. Ich würde aber auch nichts gegen die Vormittagsstunde 11 Uhr zu erinnern haben. Ich setze übrigens voraus, daß das Examen nicht vor der nächsten Woche statt finden wird.

Gauß.

The manuscript submitted by Riemann is a testament of the thorough and deep studies by the author in the area to which the treated subject belongs; of an aspiring and truly mathematical research spirit, and of a glorious, productive self-activity. The presentation is comprehensive and concise, partly even elegant: the major part of the readers would however in some parts still wish for more transparency and better arrangement. As a whole, it is a dignified valuable work, which does not only satisfy the requirement one usually imposes on a manuscript to obtain a PhD degree, but goes very far beyond.

The mathematics exam I will do myself. I prefer Sunday or Friday, and in the afternoon at 5 or 5:30 pm. I would also be available in the morning at 11am. I assume that the exam will not be before next week.

*** R. Remmert. Funktionentheorie. Springer, 1991.**

The Riemann Mapping Theorem

- Riemann's thesis contained the foundation of analytic function theory.
- This included the Riemann Mapping Theorem:

> "Two simply connected surfaces can always be mapped one to the other, such that each point on the former moves continuously with the point on the latter…"

- Riemann gave a constructive proof:
  - We need to find an analytic function f which maps Ω to the unit disk and one point $z_0 \in \Omega$ into 0. We thus set $f(z) := (z-z_0)\, e^{g(z)}$, where $g=u+iv$ is an analytic function to be determined, in order to ensure that z_0 is the only point mapped into zero.
  - In order to arrive from the boundary $\partial\Omega$ to the boundary of the disk with the mapping, we must have for all $z \in \partial\Omega$ that $|f(z)|=1$, which implies that
    $$1 = |f(z)| = |(z-z_0)e^{u+iv}| = |(z-z_0)|e^u \Rightarrow u(z) = -\log|z-z_0|,\ \forall z \in \partial\Omega$$
  - Since g is analytic, the real part u of g satisfies Laplace's equation $\nabla^2 u = 0$ on Ω, with the boundary values given above.
  - It thus suffices to solve for u, construct v using the Cauchy-Riemann equations,
    $$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} = \frac{\partial \mathbf{v}}{\partial \mathbf{y}},\ \frac{\partial \mathbf{u}}{\partial \mathbf{y}} = -\frac{\partial \mathbf{v}}{\partial \mathbf{x}}$$
    and then the construction of f is complete.

The Riemann Mapping Theorem

- But there's a problem: Riemann assumed that a solution to Laplace's equation on an arbitrary domain with given boundary conditions exists. Was that really true?
- When confronted with this question, Riemann said *

> "To this end, one can often invoke a principle for finding a function that solves Laplace's equation, which Dirichlet has been using in his lectures over the past few years."

- Riemann called this "Dirichlet's Principle".
- Suppose we want to minimize

$$\mathbf{E[u(x,y)]} = \iint_{\Omega} \mathbf{f\left(x, y, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) dxdy}$$

where u(x,y) takes on a specified value on ∂Ω. The solution must satisfy the Euler-Lagrange equation

$$\frac{\partial \mathbf{f}}{\partial \mathbf{u}} - \frac{\partial}{\partial \mathbf{x}} \frac{\partial \mathbf{f}}{\partial \mathbf{u_x}} - \frac{\partial}{\partial \mathbf{y}} \frac{\partial \mathbf{f}}{\partial \mathbf{u_y}} = \mathbf{0}$$

- As a specific example, suppose

$$\mathbf{f(x,y)} = \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^2 + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{y}}\right)^2$$

- Then, the Euler-Lagrange equation reduces to Laplace's equation, $\nabla^2 \mathbf{u(x,y)} = \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + \frac{\partial^2 \mathbf{u}}{\partial \mathbf{y}^2} = \mathbf{0}$

*** Berhard Riemann. Grundlagen fur eine allgemeine Theorie der Functionen einer veranderlichen complexen Grosse. PhD thesis, Gottingen, 1851. Werke p. 3-34, transcribed by D. R. Wilkins, April 2000.**

The Riemann Mapping Theorem

- Riemann inferred the existence of a function u(x,y) from the fact that it would be the solution to a well-defined problem in the calculus of variations.
- The calculus of variations thus became a ***guarantor*** for the existence of a function needed for the Riemann mapping theorem.*
- But do all problems in the calculus of variations have a solution? Weierstrass provided this example:

$$\min \int_{-1}^{1} \left(x \frac{\partial u}{\partial x} \right)^2 dx, \quad u(-1)=a,\ u(1)=b$$

- The integrand is strictly positive. To make the function small, u(x) can only have a large derivative near x=0. One can make the function arbitrarily small, but the minimum of zero can be achieved only for a step function, which is not differentiable.
- Weierstrass said [1869],**

> "Dirichlet's reasoning apparently leads to an incorrect result in this case."

- Undaunted, Riemann said,**

> "... my existence theorems nevertheless hold."

- Helmholtz interjected,**

> "For us physicists the Dirichlet principle remains a proof."

*** Hans Niels Jahnke, A History of Analysis, (History of Mathematics, V. 24), American Mathematical Society, p. 379, 2003.**
**** Felix Klein. Vorlesungen uber die Entwicklung der Mathematik im 19. Jahrhundert. Berlin, 1926. Reprinted New York 1950 and 1967.**

Dirichlet Principle or Bust?

- Weierstrass had a very bright former Ph.D. student, Hermann Schwarz (graduated 1864).
- Weierstrass suggested Schwarz investigate other means to show existence of solutions to the Laplace equation on general domains.
- For special domains, the answer had been known for quite some time:
  - Fourier (1807) for rectangular domains (using Fourier series).
  - Poisson (1815) had found the solution formula for circular domains.
- The existence of solutions of Laplace's equation on arbitrary domains appeared hopeless!

Hermann Schwarz

- **In response, Schwarz invents the first domain decomposition method! [1870]**
- His paper begins,*

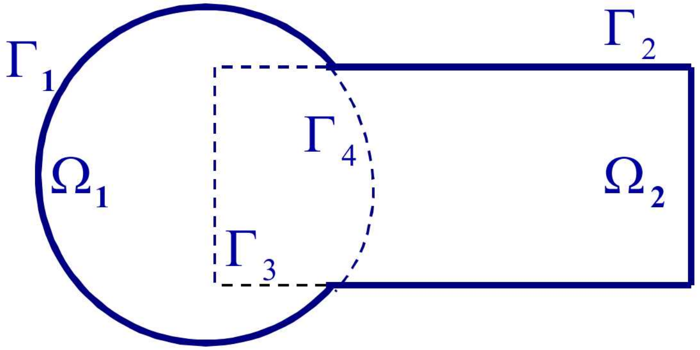
Die unter dem Namen Dirichlet'sches Princip bekannte Schlussweise, welche in gewissem Sinne als das Fundament des von Riemann entwickelten Zweiges der Theorie der analytischen Funktionen angesehen werden muss, unterliegt, wie jetzt wohl allgemein zugestanden wird, hinsichtlich der Strenge sehr begründeten Einwendungen, deren vollständige Entfernung, soviel ich weiss, den Anstrengungen der Mathematiker bisher nicht gelungen ist.

The method of conclusion, which became known under the name Dirichlet Principle, and which in a certain sense has to be considered to be the foundation of the theory of analytic functions developed by Riemann, is subject to, like it is generally admitted now, very well justified objections, whose complete removal has eluded all efforts of mathematicians to the best of my knowledge.

*** H. A. Schwarz. Uber einen Grenzubergang durch alternierendes Verfahren. Vierteljahrsschrift der Naturforschenden Gesellschaft in Zurich, 15:272–286, Mai 1870.**

Alternating Schwarz

- Since solutions to the Laplace equation were shown to exist on rectangles and circles (no Dirichlet Principle needed), Schwarz considered this shape:



- Schwarz proposed the following iterative process, and showed it converged.

1. Let $\mathbf{u}_1^{(0)} = \mathbf{0}, \mathbf{u}_2^{(0)} = \mathbf{0}$.
2. For i=1,2,…

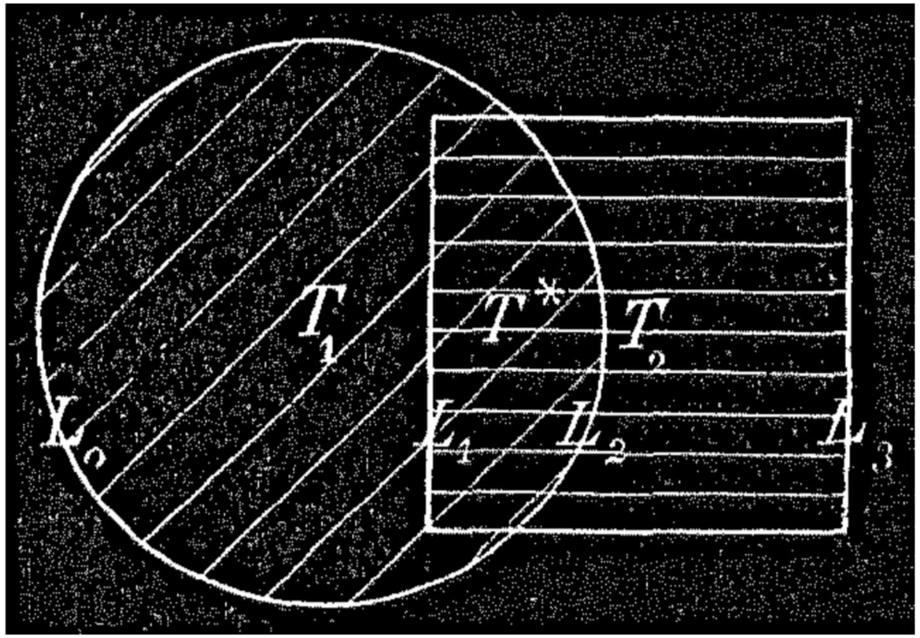
Solve $\begin{cases} \nabla^2 \mathbf{u}_1^{(i)} = \mathbf{0} \text{ on } \Omega_1 \\ \mathbf{u}_1^{(i)} = \mathbf{g} \text{ on } \Gamma_1 \\ \mathbf{u}_1^{(i)} = \mathbf{u}_2^{(i-1)} \text{ on } \Gamma_4 \end{cases}$

Solve $\begin{cases} \nabla^2 \mathbf{u}_2^{(i)} = \mathbf{0} \text{ on } \Omega_2 \\ \mathbf{u}_2^{(i)} = \mathbf{g} \text{ on } \Gamma_2 \\ \mathbf{u}_2^{(i)} = \mathbf{u}_1^{(i)} \text{ on } \Gamma_3 \end{cases}$

- Since the process converges, the converged value must be the solution of Laplace's equation on Ω.
- Adding other circles or rectangles Schwarz then proved recursively the existence of solution for more and more complicated domains.
- This closed the gap in Riemann's proof.

Alternating Schwarz

- Schwartz thought about this process very mechanically.



Schwarz's original drawing from his 1870 paper

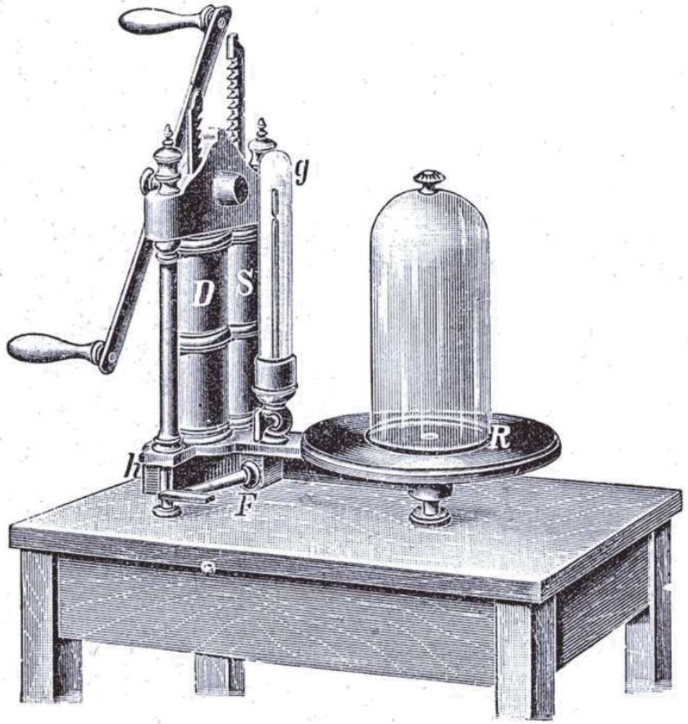


Fig. 103. Zweistiefelige Hahnluftpumpe

Schwarz's physical interpretation of the method using a two level vacuum pump

Alternating Schwarz

Other significant contributions:

- Sobolev[1] gave a variational convergence proof for the case of elasticity (1936).
- This became a practical computational method with the advent of two-level additive Schwartz[5] (1987).
- P.L. Lions[2,3,4] has a series of publications that greatly expanded the theory (1988-89).

[1] S. L. Sobolev. L'Algorithme de Schwarz dans la Th´eorie de l'Elasticit´e. Comptes Rendus (Doklady) de l'Acad´emie des Sciences de l'URSS, IV((XIII) 6):243–246, 1936.
[2] Pierre-Louis Lions. On the Schwarz alternating method. I. In Roland Glowinski, Gene H. Golub, Gerard A. Meurant, and Jacques Periaux, editors, First International Symposium on Domain Decomposition Methods for Partial Differential Equations, pages 1–42, Philadelphia, PA, 1988. SIAM.
[3] Pierre-Louis Lions. On the Schwarz alternating method II: Stochastic interpretation and orders properties. In Tony Chan, Roland Glowinski, Jacques Periaux, and Olof Widlund, editors, Domain Decomposition Methods, pages 47–70, Philadelphia, PA, 1989. SIAM.
[4] Pierre-Louis Lions. On the Schwarz alternating method III: A variant for nonoverlapping subdomains. In Tony F. Chan, Roland Glowinski, Jacques Periaux, and Olof Widlund, editors, Third International Symposium on Domain Decomposition Methods for Partial Differential Equations, held in Houston, Texas, March 20-22, 1989, pages 202–223, Philadelphia, PA, 1990. SIAM.
[5] Maksymilian Dryja and Olof B. Widlund. An additive variant of the Schwarz alternating method for the case of many subregions. Technical Report 339, also Ultracomputer Note 131, Department of Computer Science, Courant Institute, 1987.

Domain Decomposition

Historical and Mathematical Origins

Convergence Analysis

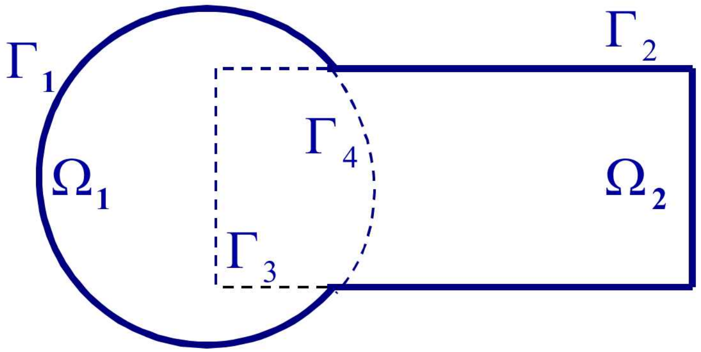
Multiscale Modeling: Atomistic-to-Continuum Coupling

Multi-Model Coupling: Classical Elasticity and Peridynamics

Alternating Schwarz: Convergence Proof

- Theorem[1]: Alternating Schwarz converges to the solution of the global problem,

$$\begin{aligned} \nabla^2 \mathbf{u} &= \mathbf{0} \text{ on } \Omega_1 \cup \Omega_2 \\ \mathbf{u} &= \mathbf{g} \text{ on } \Gamma_1 \cup \Gamma_2 \end{aligned}$$



Let u denote the solution to the global problem. Then, there exist $C_1, C_2 \in (0,1)$ such that for all $i \geq 0$

- $\left\| u_{|\Omega_1} - u_1^{(i+1)} \right\|_{L^\infty(\Omega_1)} \leq C_1^{(i)} C_2^{(i)} \left\| u - u^{(0)} \right\|_{L^\infty(\Gamma_4)}$
- $\left\| u_{|\Omega_2} - u_2^{(i+1)} \right\|_{L^\infty(\Omega_2)} \leq C_1^{(i+1)} C_2^{(i)} \left\| u - u^{(0)} \right\|_{L^\infty(\Gamma_3)}$

- C_1, C_2 depend on size of overlap and can be very close to one if overlap small.

1. Let $\mathbf{u}_1^{(0)} = \mathbf{0}, \mathbf{u}_2^{(0)} = \mathbf{0}$.
2. For i=1,2,…

Solve $\begin{cases} \nabla^2 \mathbf{u}_1^{(i)} = \mathbf{0} \text{ on } \Omega_1 \\ \mathbf{u}_1^{(i)} = \mathbf{g} \text{ on } \Gamma_1 \\ \mathbf{u}_1^{(i)} = \mathbf{u}_2^{(i-1)} \text{ on } \Gamma_4 \end{cases}$

Solve $\begin{cases} \nabla^2 \mathbf{u}_2^{(i)} = \mathbf{0} \text{ on } \Omega_2 \\ \mathbf{u}_2^{(i)} = \mathbf{g} \text{ on } \Gamma_2 \\ \mathbf{u}_2^{(i)} = \mathbf{u}_1^{(i)} \text{ on } \Gamma_3 \end{cases}$

[1] A. Quarteroni and P.M.A. Valli, Domain Decomposition Methods for Partial Differential Equations, Clarendon Press, 1999, p. 27.

Sidebar: Condition Number

We denote the condition number of A as $\kappa(\mathrm{A}) := \|\mathrm{A}\|\|\mathrm{A}^{-1}\|$.

We can demonstrate its usefulness via perturbation analysis. Let Au=f and consider the perturbed system:

- $(\mathrm{A} + \varepsilon\mathrm{E})\mathrm{x}(\varepsilon) = \mathrm{b} + \varepsilon\mathrm{e}$

Let $\delta(\varepsilon) = \mathrm{x}(\varepsilon) - \mathrm{x}$. Then,

- $(\mathrm{A} + \varepsilon\mathrm{E})\delta(\varepsilon) = \mathrm{b} + \varepsilon\mathrm{e} - (\mathrm{b} - \varepsilon\mathrm{E})$
- $(\mathrm{A} + \varepsilon\mathrm{E})\delta(\varepsilon) = \varepsilon(\mathrm{e} - \mathrm{Ex})$
- $\delta(\varepsilon) = \varepsilon(\mathrm{A} + \varepsilon\mathrm{E})^{-1}\,(\mathrm{e} - \mathrm{Ex})$

We observe that the function $\mathrm{x}(\varepsilon)$ is differentiable at ε=0:

- $\mathrm{x}'(0) = \lim_{\varepsilon\to 0} \frac{\mathrm{x}(0+\varepsilon)-\mathrm{x}(0)}{\varepsilon} = \mathrm{A}^{-1}\,(\mathrm{e} - \mathrm{Ex})$

Perturbing the pair (A,b) by the small amount (εE,εe) will cause the solution to change by $\varepsilon\mathrm{x}'(0)$. Thus,

- $\|\mathrm{x}(\varepsilon) - \mathrm{x}\| = \varepsilon\|\mathrm{A}^{-1}\,(\mathrm{e} - \mathrm{Ex})\|$
- $\|\mathrm{x}(\varepsilon) - \mathrm{x}\| \leq \varepsilon\|\mathrm{A}^{-1}\|(\|\mathrm{e}\| + \|\mathrm{E}\|\|\mathrm{x}\|) + O(\varepsilon^2)$

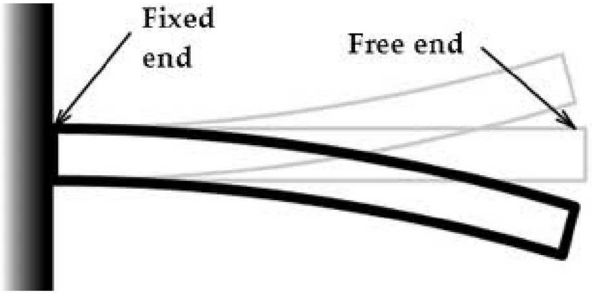
Further simplification and use of the relationship $\|\mathrm{b}\| \leq \|\mathrm{A}\|\|\mathrm{x}\|$ gives the relative variation in the solution to the relative sizes of the perturbation

- $\frac{\|\mathrm{x}(\varepsilon)-\mathrm{x}\|}{\|\mathrm{x}\|} \leq \varepsilon\|\mathrm{A}^{-1}\|\|\mathrm{A}\|\left(\frac{\|\mathrm{e}\|}{\|\mathrm{b}\|} + \frac{\|\mathrm{E}\|}{\|\mathrm{A}\|}\right) + O(\varepsilon^2)$

Sidebar: Condition Number

What does this mean physically?

- For Ill-conditioned systems, small perturbation in input can result in a large change in solution

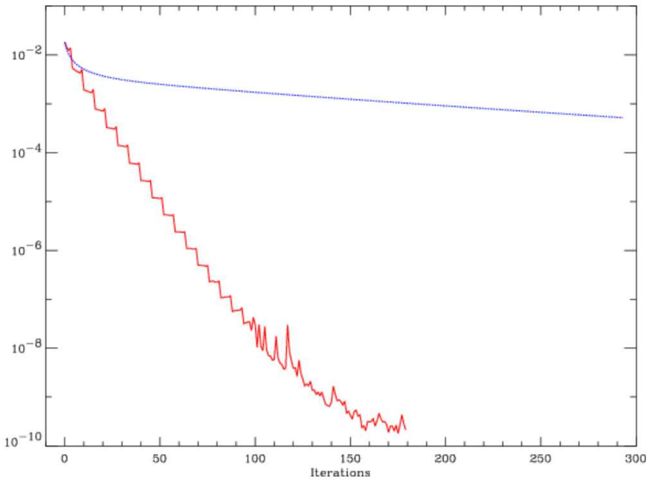


Cantilevered beam

What does this mean for linear solvers?

- Condition number dictates accuracy
  - Using relationships Ax=b, e=A^{-1}r, can show that $\frac{\|e\|}{\|x\|} \leq \|A\|\|A^{-1}\|\frac{\|r\|}{\|b\|}$
  - Small relative residual does not imply small relative error!

- Condition number dictates convergence rate
  - Convergence rate of conjugate gradients: $\|e^{(k)}\|_A \leq 2\left(\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}\right)^k \|e^{(0)}\|_A$



Convergence curves for optimal Krylov methods

Sidebar: Structure of a Simple Iterative Method

Let $Au = f$, and let $u^{(k)}$ denote an approximate solution at iteration k.
Let $e^{(k)} = u - u^{(k)}$ and $r^{(k)} = f - Au^{(k)}$ denote the error and residual at iteration k, respectively.

Suppose $A = M - N$, where M is invertable. Then,

- $Au = f$
- $(M-N)u = f$
- $Mu = Nu + f$
- $u = M^{-1}Nu + M^{-1}f$

Let this define an iteration:

- $u^{(k+1)} = (M^{-1}N)u^{(k)} + M^{-1}f$

This iteration will converge if and only if the spectral radius of the iteration matrix $M^{-1}N$ is less than one.

We can rewrite this as

- $u^{(k+1)} = (I-M^{-1}A)u^{(k)} + M^{-1}f$
  $= u^{(k)} - M^{-1}Au^{(k)} + M^{-1}f$
  $= u^{(k)} + M^{-1}(f-Au^{(k)})$
  $= u^{(k)} + M^{-1}r^{(k)}$

Form of Richardson iteration:

- $u^{(k+1)} = u^{(k)} + \tau B r^{(k)}$

Sidebar: Structure of a Simple Iterative Method

Simple iteration:

- $u^{(k+1)} = (M^{-1}N)u^{(k)} + M^{-1}f$

Thm: Convergence iff $\sigma(M^{-1}N) < 1$. Proof Sketch:

Let $e^{(k)} = u^{(k)} - u$. Then,

- $u^{(k+1)} - u = (M^{-1}N)u^{(k)} + M^{-1}f - u$
- $e^{(k+1)} = (M^{-1}N)u^{(k)} + M^{-1}Au - u$
- $e^{(k+1)} = (M^{-1}N)u^{(k)} + M^{-1}(M-N)u - u$
- $e^{(k+1)} = (M^{-1}N)u^{(k)} + (I-M^{-1}N)u - u$
- $e^{(k+1)} = (M^{-1}N)u^{(k)} - (M^{-1}N)u$
- $e^{(k+1)} = (M^{-1}N)e^{(k)}$
- $e^{(k+1)} = (M^{-1}N)^k e^{(0)}$

Let $M^{-1}N = V\Lambda V^{-1}$, where $\sigma(M^{-1}N) = |\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|$. Then,

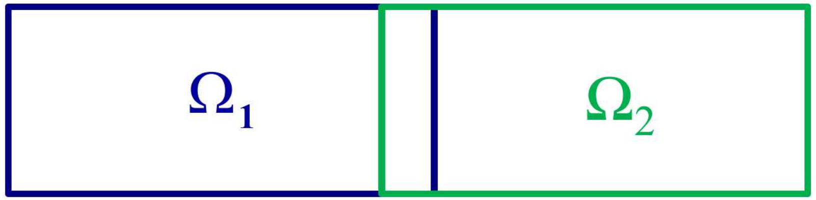
- $e^{(k+1)} = (M^{-1}N)^k e^{(0)} = V\Lambda^k V^{-1} e^{(0)} = \sum_{i=1}^{n} v_i \lambda_i^k \eta_i$, where $\eta = V^{-1}e^{(0)}$
- $e^{(k+1)} = v_1\lambda_1^k\eta_1 + \sum_{i=2}^{n} v_i\lambda_i^k\eta_i$
- $e^{(k+1)} = \lambda_1^k \left(v_1\eta_1 + \sum_{i=2}^{n} v_i \left(\frac{\lambda_i}{\lambda_1}\right)^k \eta_i \right)$

Thus, for $k \gg 1$,

- $\frac{\|e^{(k+1)}\|}{\|e^{(k)}\|} \approx \lambda_1 = \sigma(M^{-1}N)$

Alternating Schwarz is a Simple Iteration

- Consider the two-subdomain problem



- Let the global problem be $Au=f$.
- Let R_i, $i=1,2$ be a rectangular restriction matrix that returns unknowns defined in $\Omega_{i.}$

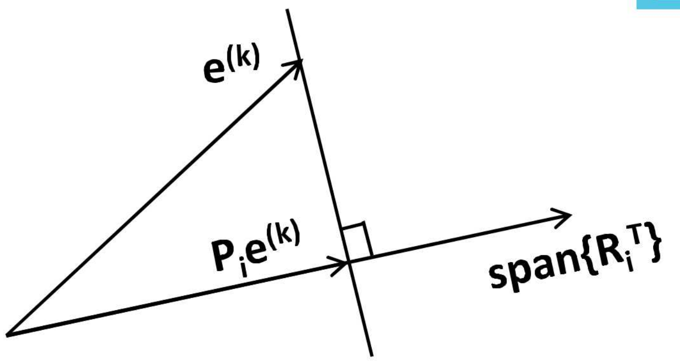
- We can write alternating Schwarz as
  - $u^{(k+1/2)} = u^{(k)} + R_1^T(R_1 A R_1^T)^{-1} R_1 r^{(k)}$
  - $u^{(k+1)} \;\; = u^{(k+1/2)} + R_2^T(R_2 A R_2^T)^{-1} R_2 r^{(k)}$

- Let $B_i = R_i^T(R_i A R_i^T)^{-1} R_i$. We can re-write Alternating Schwarz as
  - $u^{(k+1)} \;\; = u^{(k)} + (B_1 + B_2 + B_2AB_1)\, r^{(k)}$

- This takes the form of a simple iteration. The B_i are orthogonal projectors.
- Defining $P_1=B_1A$, $P_2=B_2A$, and noting that $e^{(k)} = A^{-1}r^{(k)}$, we can rewrite the iteration as
  - $e^{(k+1)} \;\; = [I - (P_1 + P_2 - P_2P_1)]\, e^{(k)}$

- As before, this iteration will converge iff the spectral radius of the iteration matrix is less than one.

Alternating Schwarz is a Simple Iteration



Alternating Schwarz takes the form

- $e^{(k+1)} = [I - (P_1 + P_2 - P_2 P_1)]\, e^{(k)}$

Note that

- $P_i = P_i^2$ (i.e., P is a projector)

If A is SPD, then

- $(P_i\, x, y)_A = x^T P_i^T A\, y = x^T A\, B_i\, A\, y = x^T A\, P_i\, y = (x, P_i\, y)_A$
- i.e., P_i is an orthogonal projector in the A-norm onto $V_i = \mathrm{span}\{R_i^T\}$

This suggests (geometrically) that each projected error is smaller than the last.

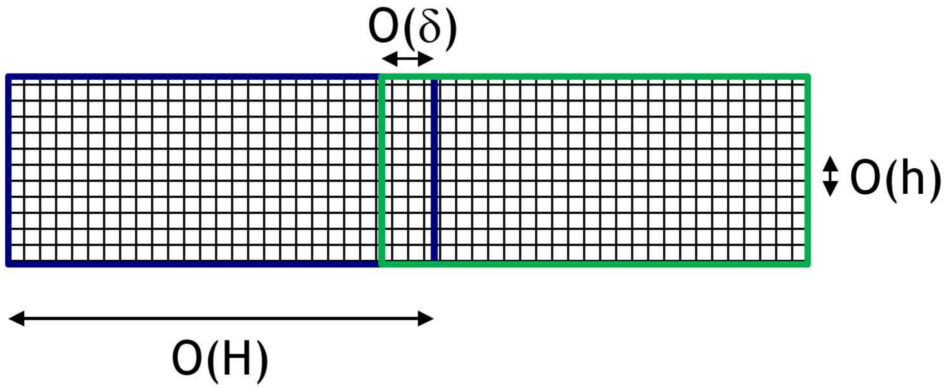
Key observation: Alternating Schwarz proceeds by:

1. Restriction: R_i
2. Solution of a (smaller) linear system $(R_i\, A\, R_i^T)\, u_i = f_i$
3. Prolongation: R_i^T

This process is fundamental to all domain decomposition and multigrid/multilevel algorithms.

Alternating Schwarz is a Simple Iteration

Convergence behavior of Schwarz



- $\kappa(A) \leq C/h^2$
- $\kappa(P^{-1}A) \leq C/(\delta^2 H^2)$ [1]

This means:[2]

- The number of iterations grows as H decreases
- If δ ~ H and H is fixed, the number of iterations is bounded independent of h. This means the behavior of the discrete problem is like the continuous problem: If the number of subdomains is fixed, the number of Schwarz iterations does not vary with h (assuming exact subdomain solves).
- Convergence is poor for small δ.

[1] A. Quarteroni and P.M.A. Valli, Domain Decomposition Methods for Partial Differential Equations, Clarendon Press, 1999, p. 95.
[2] B. Smith, P. Bjorstad, W. Gropp, Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations, Cambridge University Press, 1996, p. 24.

Domain Decomposition

Historical and Mathematical Origins

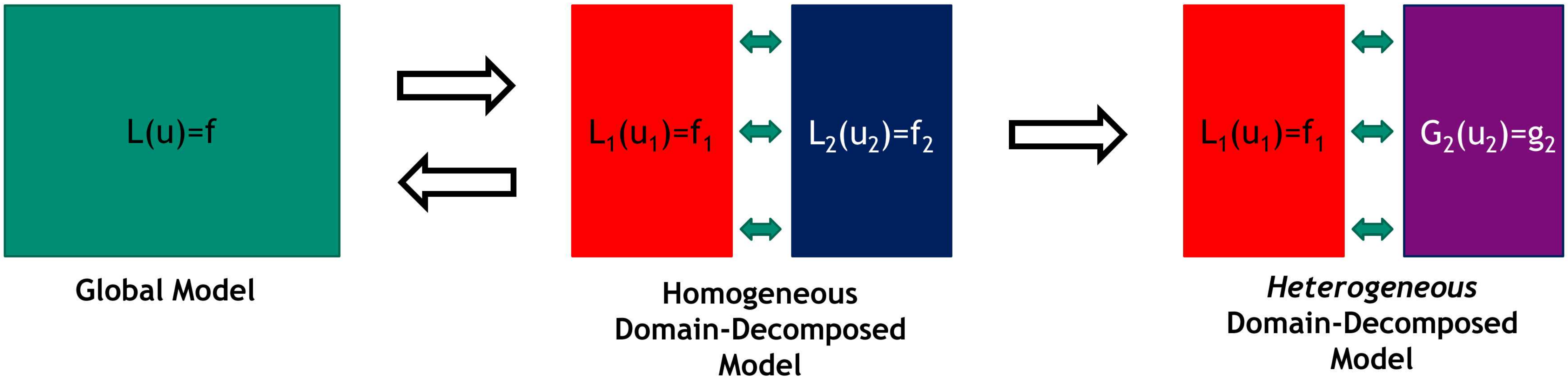
Convergence Analysis

Multiscale Modeling: Atomistic-to-Continuum Coupling

Multi-Model Coupling: Classical Elasticity and Peridynamics

Heterogeneous Domain Decomposition

- Domain decomposition methods all assume the existence of some global problem to be solved, and show how to break it into subdomains.
- Each subdomain knows about the other subdomains only through its boundary.
- This presents the opportunity to substitute out one subdomain with *a completely different model*, and provides an algorithmic framework for mathematically consistent multi-model coupling.



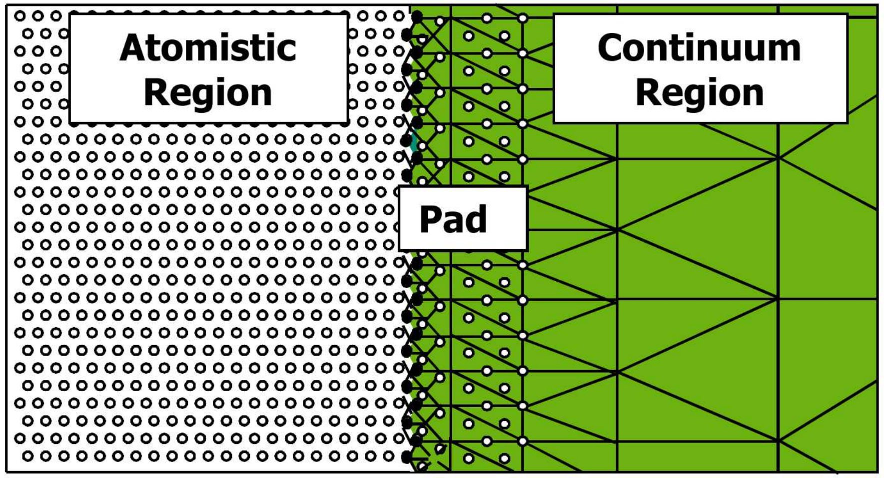
Iterative Minimization

- Write separate energy functionals for atomistic and continuum domains

- Iterate:

FE {1. Fix location of (most) pad nodes;
Minimize energy of continuum region

At {2. Fix location of (most) pad atoms;
Minimize energy of atomistic region



Cartoon of Coupled Atomistic/Continuum Model*

- This is just alternating Schwarz!

- Important difference: We do not assume existence of global equation!
- What does this mean for convergence? What does this mean for the error of the coupled model?

* W. A. Curtin and R. E. Miller, Atomistic/continuum coupling in computational materials science, Modelling Simul. Mater. Sci. Eng., 11:R33-R68, 2003.

Classical Schwarz vs. Atomistic/Continuum Schwarz

- Exploit domain decomposition theory: Overlapping Subdomain Methods (Schwarz-type)
  - Cut problem into physical subdomains
  - Solves only on each subdomain
  - Information transfer through boundary conditions

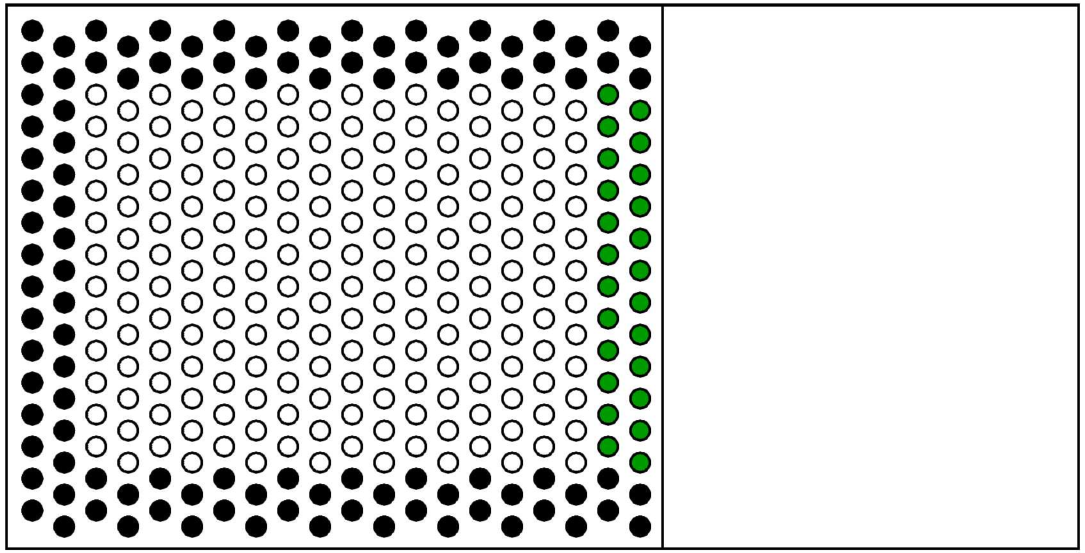
- Classical domain decomposition theory tells us:
  - Rate of convergence increases with overlap
  - Solution independent of overlap

- Still true for AtC Schwarz?

- Can I …
  - Prove convergence in AtC Schwarz case?
  - Bound rate of convergence as function of overlap?
  - Determine how solution depends on overlap?

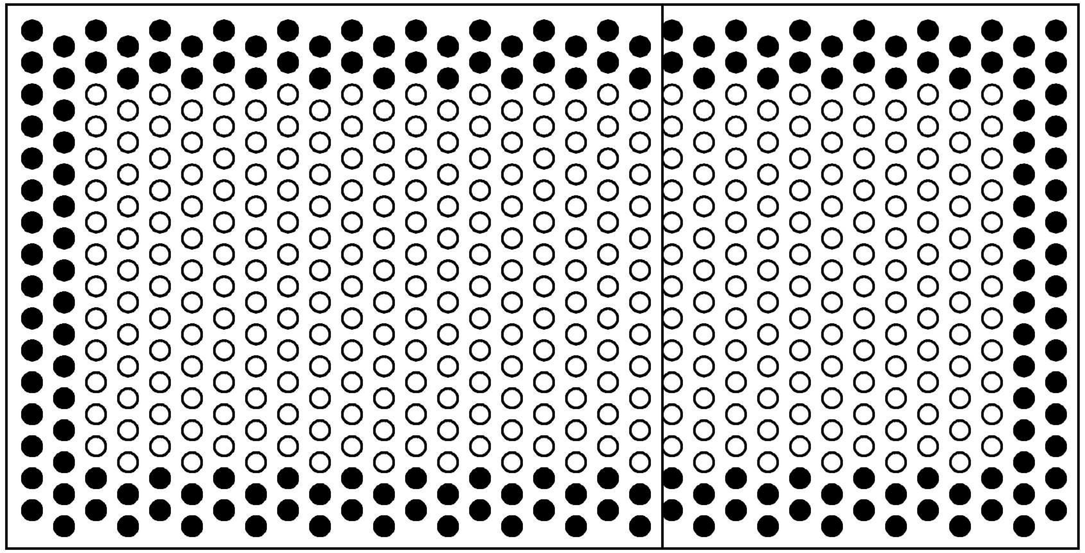
Atomistic/Continuum Schwarz

- Assume regular (Bravais-like) atomic lattice (1D, 2D, 3D)
- Assume At and FE couple same material



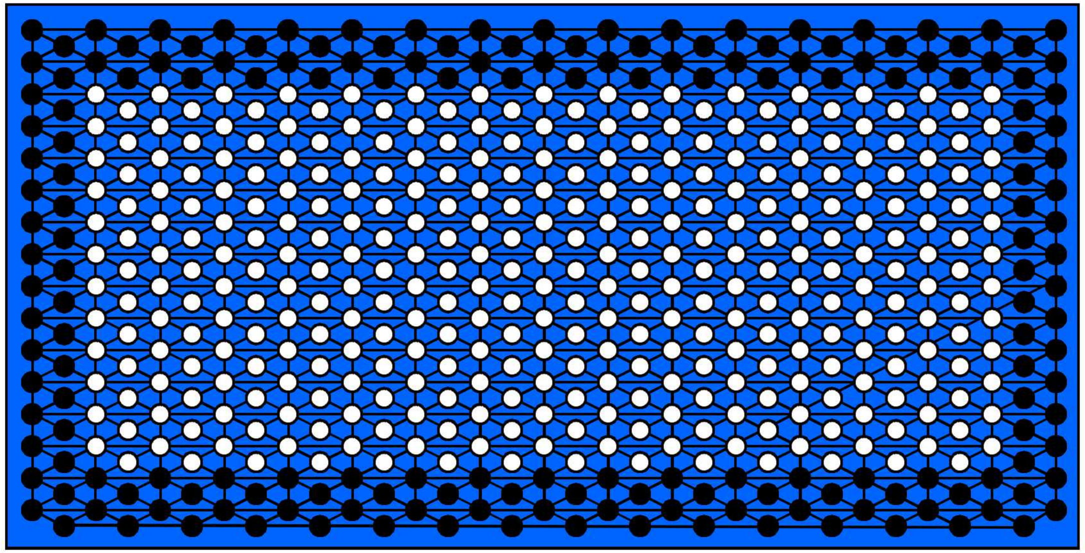
Atomistic/Continuum Schwarz

- Assume atomic lattice extends into FE domain (this defines global atomistic model)



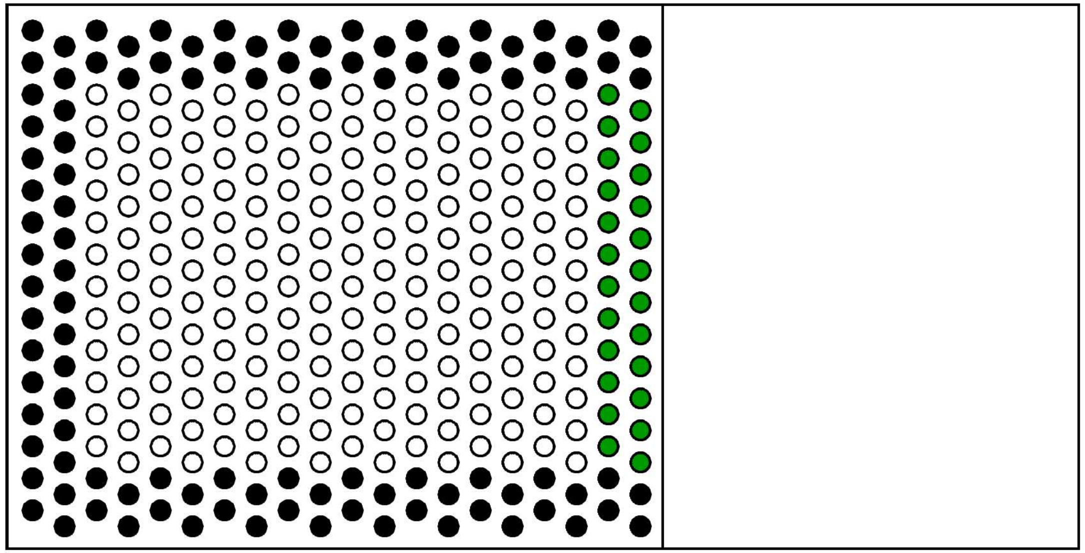
Atomistic/Continuum Schwarz

- Assume atomic lattice extends into FE domain (this defines global atomistic model)
- Use lattice to define FE mesh (this defines global finite element model)



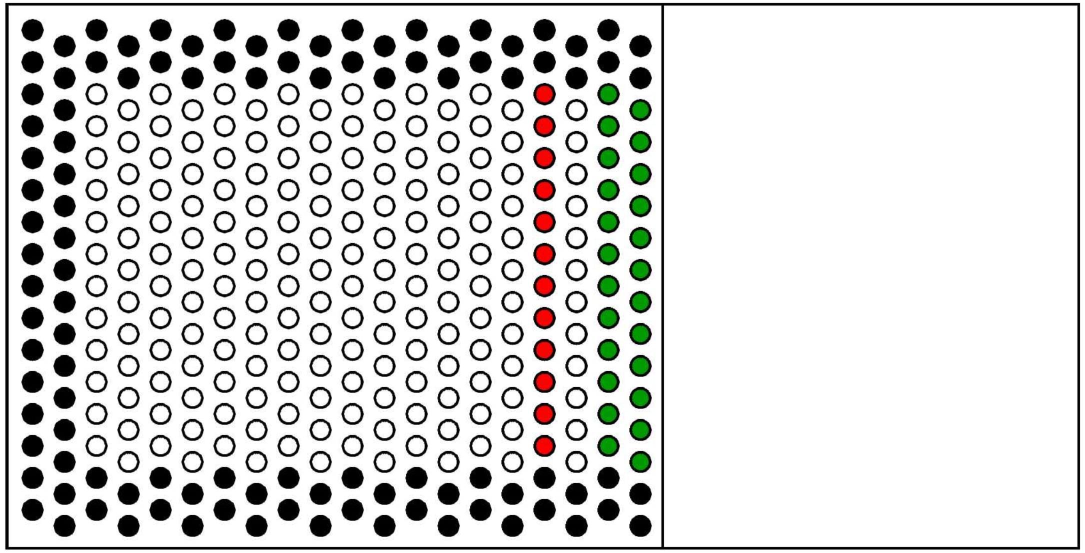
Atomistic/Continuum Schwarz

- Step #1: Solve atomistic problem



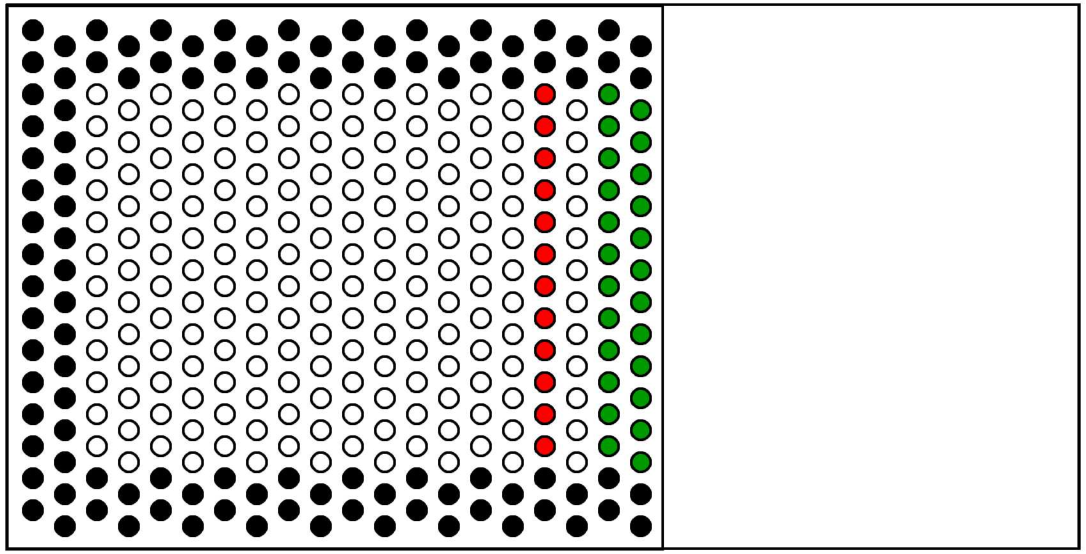
Atomistic/Continuum Schwarz

- Step #1: Solve atomistic problem
  - Record new positions for all unconstrained atoms



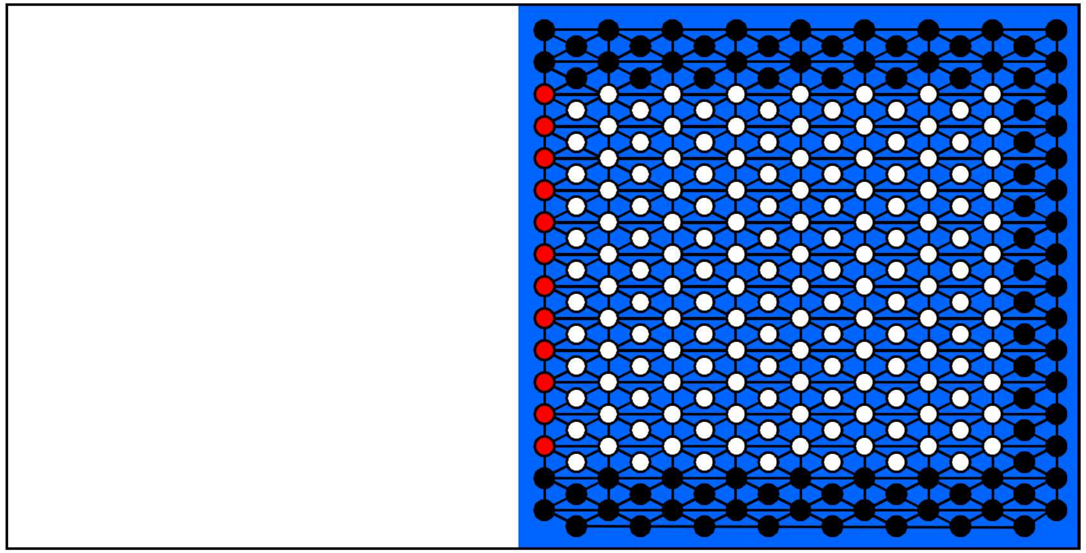
Atomistic/Continuum Schwarz

- Step #1: Solve atomistic problem
  - Record new positions for all unconstrained atoms
  - Assign Dirichlet boundary conditions for FE problem



Atomistic/Continuum Schwarz

- Step #2: Solve finite element problem
  - Record new positions for all unconstrained finite element nodes
  - Assign Dirichlet boundary conditions for atomistic problem



Atomistic/Continuum Schwarz

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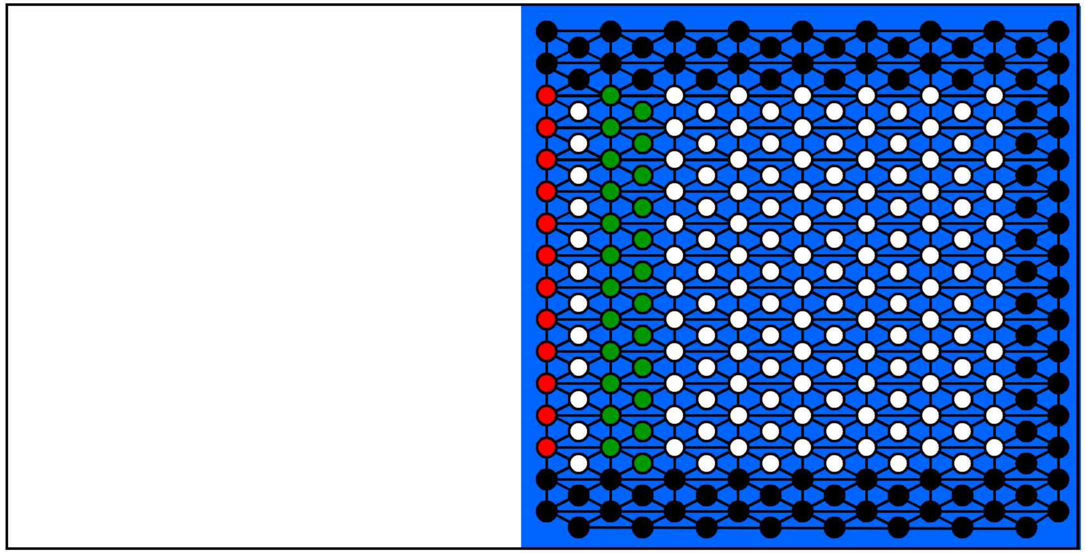

Atomistic/Continuum Schwarz

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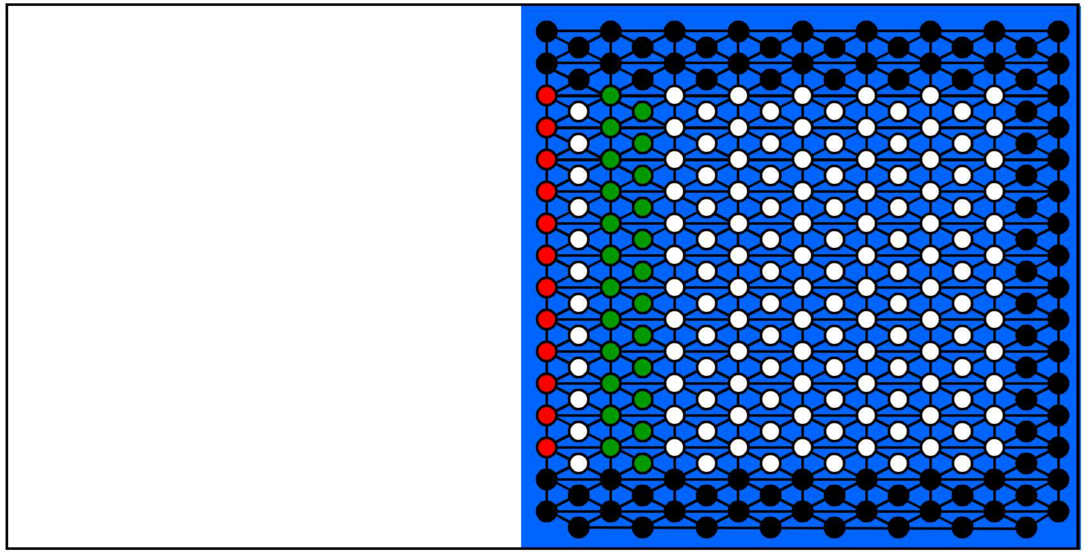

Atomistic/Continuum Schwarz

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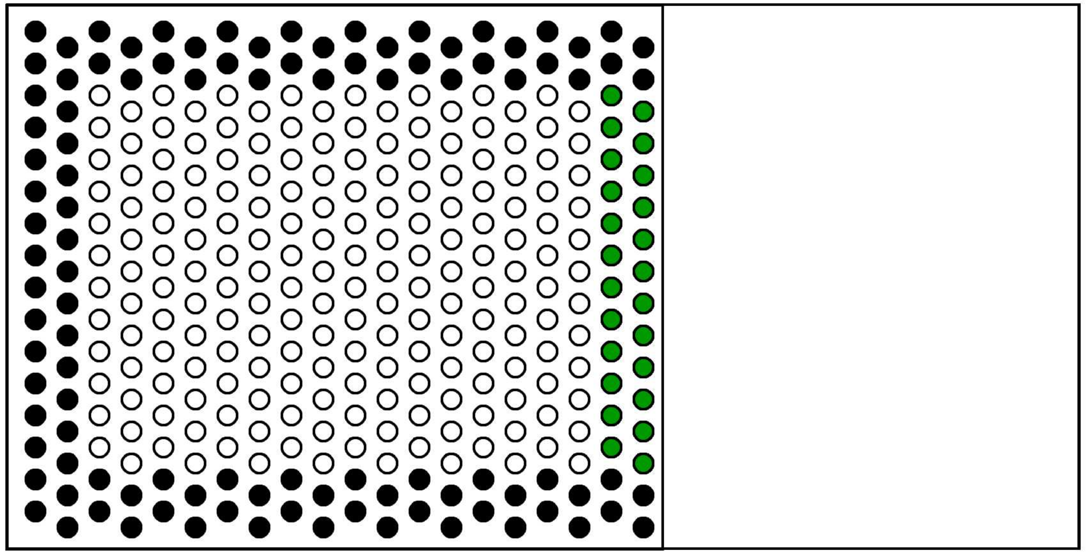
  - Record new positions for all unconstrained finite element nodes
  - Assign Dirichlet boundary conditions for atomistic problem



Atomistic/Continuum Schwarz Convergence Theory

- Let $K_C u_C$ = f (globally) and $K_A u_A$ = f (globally)
- Each AS iteration is projection of error

$$\mathbf{u}^{n+1/2} - \mathbf{u}^{n} = \mathbf{P}_A \left(\mathbf{u}_A - \mathbf{u}^{n} \right)$$

$$\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2} = \mathbf{P}_C \left(\mathbf{u}_C - \mathbf{u}^{n+1/2} \right)$$

where

$$\mathbf{P}_A = \begin{pmatrix} \left(\mathbf{K}_A^{(A)}\right)^{-1} & 0 \\ 0 & 0 \end{pmatrix} \mathbf{K}_A \qquad \mathbf{P}_C = \begin{pmatrix} \left(\mathbf{K}_C^{(C)}\right)^{-1} & 0 \\ 0 & 0 \end{pmatrix} \mathbf{K}_C$$

Atomistic/Continuum Schwarz Convergence Theory

- Let
$$\mathbf{e}_A^n = \mathbf{u}^n - \mathbf{u}_A \qquad \mathbf{u}_C = \mathbf{u}_A - \mathbf{d}$$

- Can show $\mathbf{e}_A^{n+1} = \left[\mathbf{I} - \left(\mathbf{P}_A + \mathbf{P}_C - \mathbf{P}_C\mathbf{P}_A\right)\right]\mathbf{e}_A^n + \mathbf{P}_C\mathbf{d}$

- Let $\mathbf{V}\Lambda\mathbf{V}^{-1} = \mathbf{I} - \left(\mathbf{P}_A + \mathbf{P}_C - \mathbf{P}_C\mathbf{P}_A\right)$

- Assume $0 < \sigma(\Lambda) < 1$

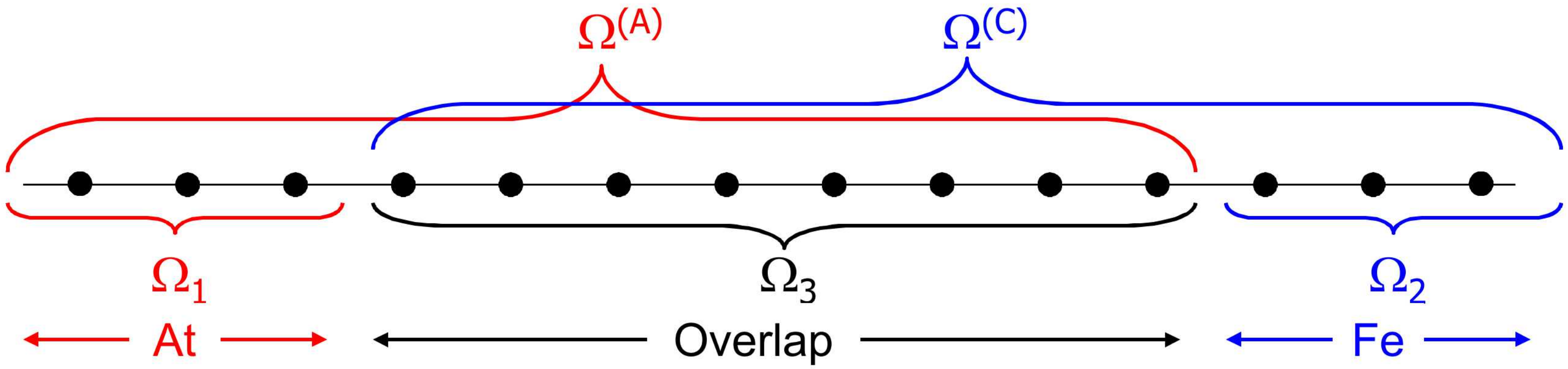
- Then

Convergence rate

$$\left\|\mathbf{e}_A^{n+1}\right\| \le \overset{\mathbf{0}}{\sigma(\Lambda)^{\mathbf{n}}}\left[\kappa(\mathbf{V})\left(\left\|\mathbf{e}_A^{\mathbf{0}}\right\| - \frac{\sigma(\Lambda)}{\mathbf{1}-\sigma(\Lambda)}\left\|\mathbf{P}_C\mathbf{d}\right\|\right)\right] + \overbrace{\left(\frac{\kappa(\mathbf{V})}{\mathbf{1}-\sigma(\Lambda)}\right)}^{\text{depends on overlap}}\overbrace{\left\|\mathbf{P}_C\mathbf{d}\right\|}^{\text{depends on models}}$$

Atomistic/Continuum Schwarz Convergence Theory

- What about $\|\mathbf{P_c d}\|$? Consider following decomposition:



- Let $\mathbf{d} = [\mathbf{d_1}\ \mathbf{d_2}\ \mathbf{d_3}]^T$ Then, $\|\mathbf{P_c d}\| \sim \|\mathbf{d_2}\|, \|\mathbf{d_3}\|$.

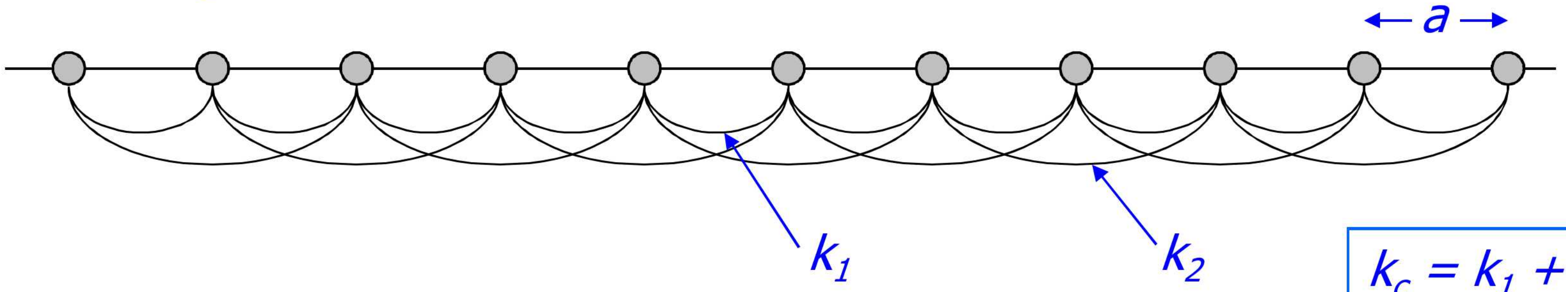
- Small error if $\|\mathbf{d_2}\|, \|\mathbf{d_3}\| \ll 1$.
- Occurs if FE solution well approximates atomistic solution in Ω_2, Ω_3 (pure continuum domain + overlap domain).

- If $\mathbf{d_2} = \mathbf{d_3} = \mathbf{0}$, can recover (global) atomistic solution!

A Simple 1D Model*

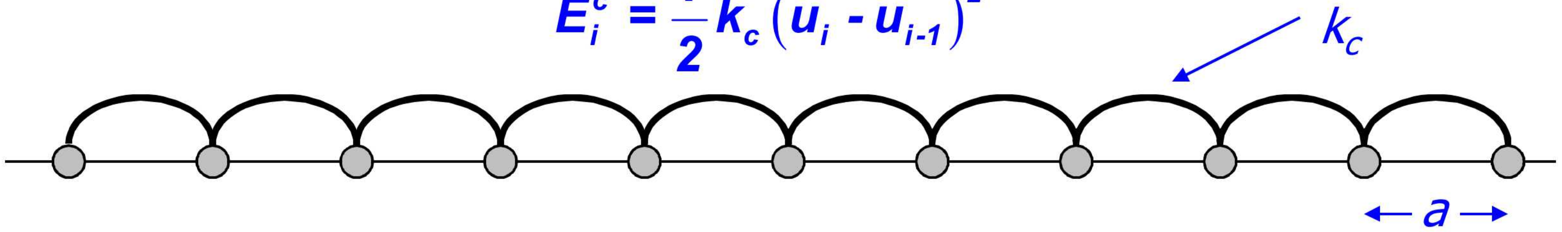
- Atomic model: Chain of 101 Atoms

$$E_i^a = \frac{1}{2}\left[\frac{1}{2}k_1\left(u_i - u_{i-1}\right)^2 + \frac{1}{2}k_1\left(u_{i+1} - u_i\right)^2 + \frac{1}{2}k_2\left(u_i - u_{i-2}\right)^2 + \frac{1}{2}k_2\left(u_{i+2} - u_i\right)^2\right]$$



$$\boxed{k_c = k_1 + 4k_2}$$

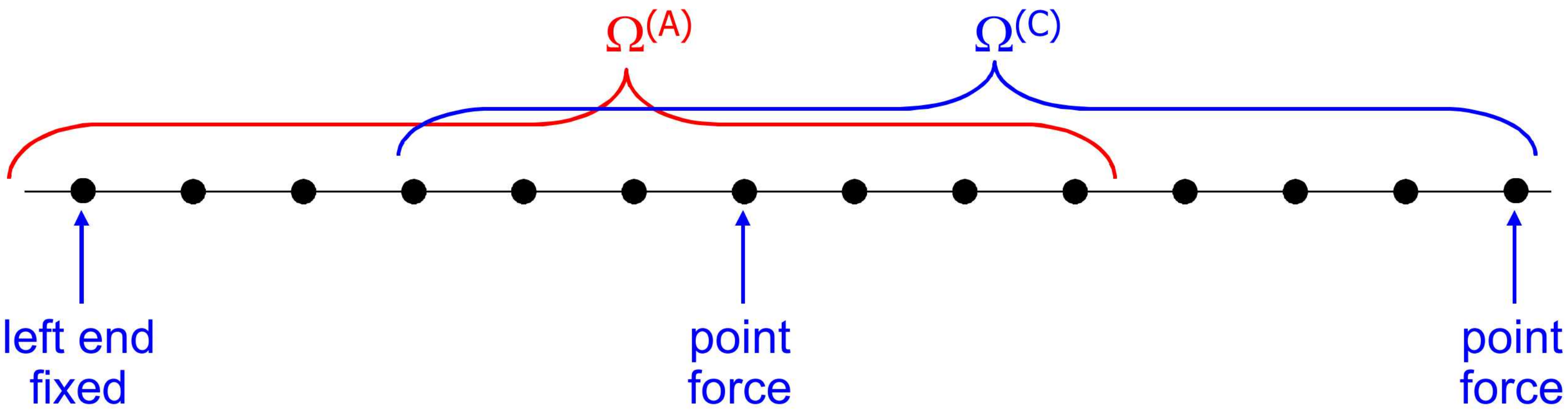
$$E_i^c = \frac{1}{2}k_c\left(u_i - u_{i-1}\right)^2$$



W. A. Curtin and R. E. Miller, Atomistic/continuum coupling in computational materials science, Modelling Simul. Mater. Sci. Eng., 11:R33-R68, 2003.

A Simple 1D Model

- Atomic model: Chain of 101 Atoms



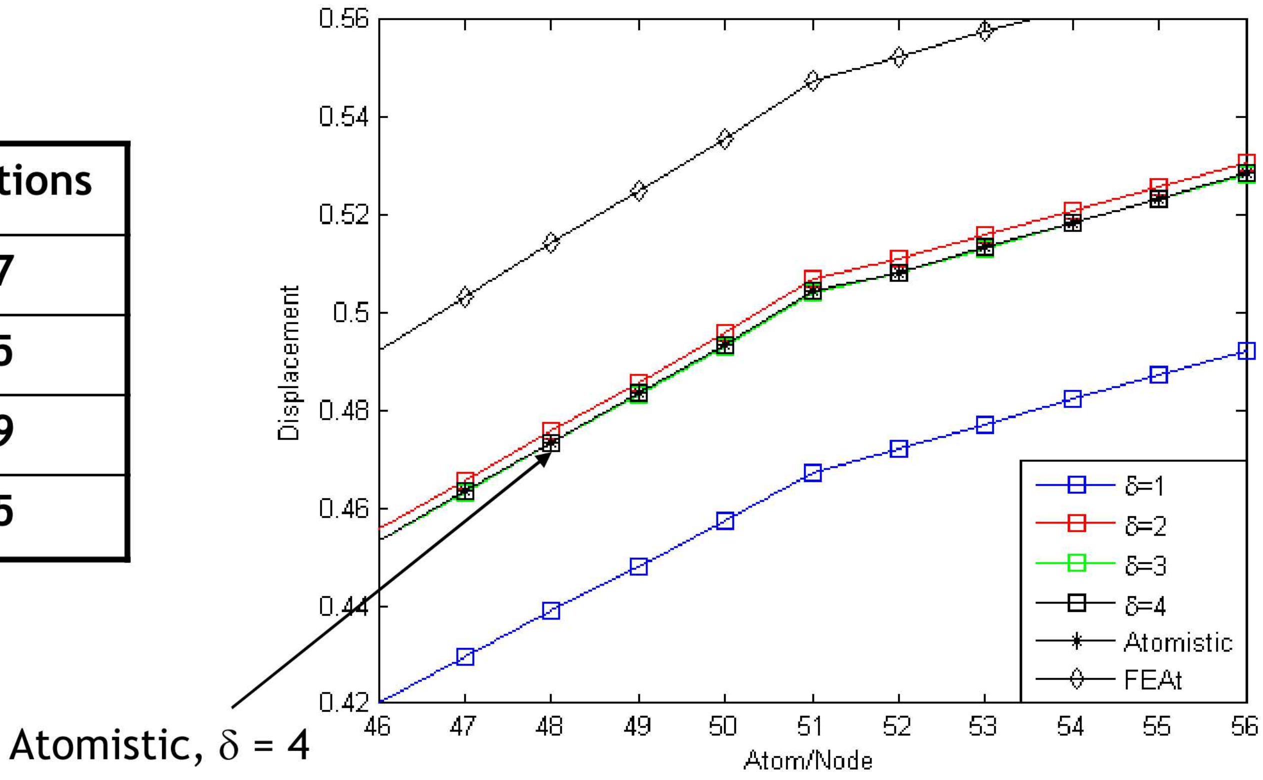
- $0 < \sigma(\Lambda) < 1$ (proof omitted)

- Vary overlap; Observe effect upon converged solution

A Simple 1D Model

- Left atom fixed; Force applied to right atom and atom 51
- # Iterations decreases with increasing overlap
  - Expected from DD theory
  - Converge to atomistic solution

δ	$\sigma(\Lambda)$	# Iterations
1	0.9551	387
2	0.8840	145
3	0.8173	89
4	0.7555	65



Domain Decomposition

Historical and Mathematical Origins

Convergence Analysis

Multiscale Modeling: Atomistic-to-Continuum Coupling

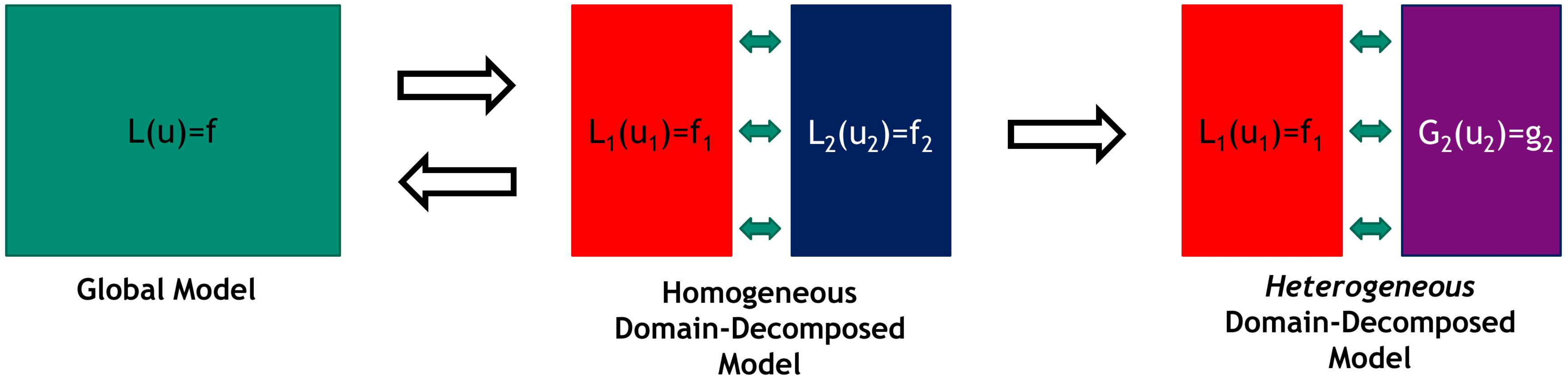
Multi-Model Coupling: Classical Elasticity and Peridynamics

Heterogeneous Domain Decomposition

- Domain decomposition methods all assume the existence of some global problem to be solved, and show how to break it into subdomains.

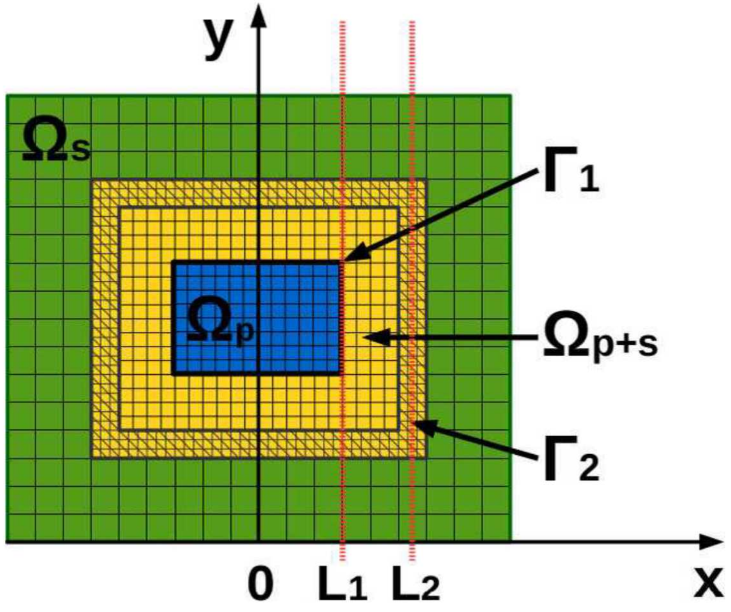
- Each subdomain knows about the other subdomains only through its boundary.

- This presents the opportunity to substitute out one subdomain with *a completely different model*, and provides an algorithmic framework for mathematically consistent multi-model coupling.



Local/Nonlocal Coupling*

- Classical linear elasticity is a local model
  - $\nabla \cdot \mathbf{S}(\mathbf{u}_s(\mathbf{x})) + \mathbf{b}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Omega_s$
  - $\mathbf{S}(\mathbf{u}_s(\mathbf{x})) = \frac{\upsilon E}{2(1+\upsilon)(1-2\upsilon)}\left[\mathrm{tr}\left(\left(\frac{\partial \mathbf{u}_s}{\partial \mathbf{x}}\right) + \left(\frac{\partial \mathbf{u}_s}{\partial \mathbf{x}}\right)^{\mathbf{T}}\right)\right] + \frac{E}{(1+2\upsilon)}\left[\left(\frac{\partial \mathbf{u}_s}{\partial \mathbf{x}}\right) + \left(\frac{\partial \mathbf{u}_s}{\partial \mathbf{x}}\right)^{\mathbf{T}}\right]$



- Peridynamics is a nonlocal model
  - $\int_{H_x} \mathbf{f}(\mathbf{u}_p(\mathbf{x}') - \mathbf{u}_p(\mathbf{x}), \mathbf{x}' - \boldsymbol{x})\boldsymbol{d}V_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}, \ \mathbf{x} \in \Omega_p$

- It is useful to be able to couple these models using only black-box codes to leverage each model where it is of most value.

* Y. Yu, F. F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations, CMAME, 340, 2018, pp. 905-931.

Local/Nonlocal Coupling*

- Solve the coupled system using Alternating Schwarz

- Boundary Conditions for Linear Elastic Domain
  - Dirichlet: $\mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x}) = \mathbf{u}_{\mathrm{p}}^{\mathrm{n}-\mathbf{1}}(\mathbf{x}), \ \forall\ \mathbf{x} \in \Gamma_1$
  - Neumann: $\mathbf{S}\left(\mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x})\right) \cdot \mathbf{n}_s = \mathbf{S}\left(\mathbf{u}_{\mathrm{p}}^{\mathrm{n}-\mathbf{1}}(\mathbf{x})\right) \cdot \mathbf{n}_s, \ \forall\ \mathbf{x} \in \Gamma_1$
  - Robin: $\mathbf{S}\left(\mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x})\right) \cdot \mathbf{n}_s + \mathrm{R}\mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x}) = \mathbf{S}\left(\mathbf{u}_{\mathrm{p}}^{\mathrm{n}-\mathbf{1}}(\mathbf{x})\right) \cdot \mathbf{n}_s + \mathrm{R}\mathbf{u}_{\mathrm{p}}^{\mathrm{n}-\mathbf{1}}(\mathbf{x}), \ \forall\ \mathbf{x} \in \Gamma_1$

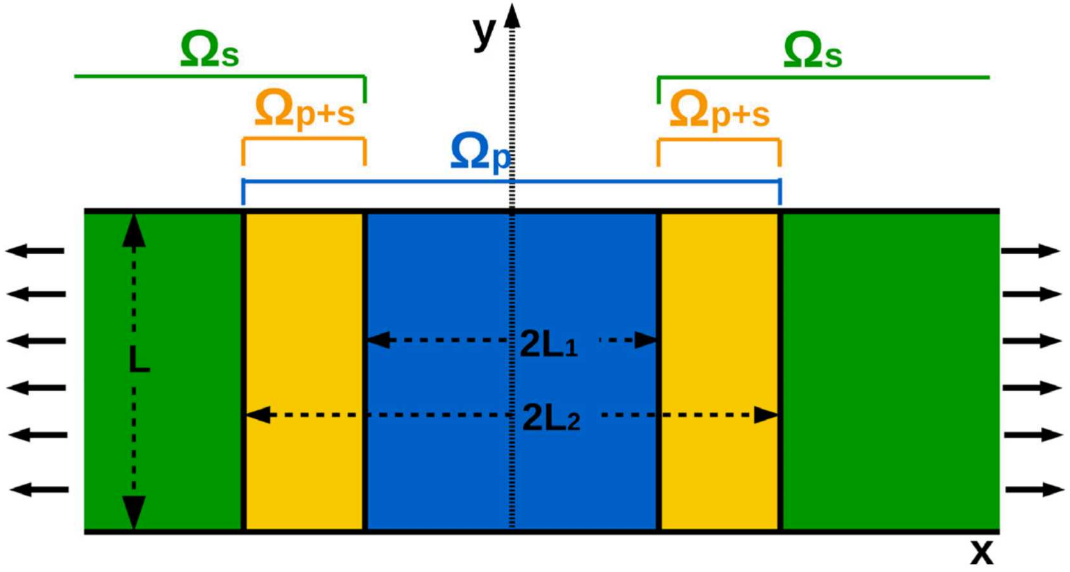
- Boundary Conditions for Peridynamic Domain
  - Dirichlet: $\mathbf{u}_{\mathrm{p}}^{\mathrm{n}}(\mathbf{x}) = \mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x}), \ \forall\ \mathbf{x} \in \Gamma_2$
  - Dirichlet w/ Aitken Acceleration: $\mathbf{u}_{\mathrm{p}}^{\mathrm{n}}(\mathbf{x}) = \tau^{\mathrm{n}}\mathbf{u}_{\mathrm{p}}^{\mathrm{n}-1}(\mathbf{x}) + (\mathbf{1} - \tau^{\mathrm{n}})\mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x}), \ \forall\ \mathbf{x} \in \Gamma_2$

$$\tau^{\mathrm{n}} = \tau^{\mathrm{n}-\mathbf{1}}\left(\tau^{\mathrm{n}-\mathbf{1}} - \mathbf{1}\right)\frac{(\mathbf{Q}^{\mathbf{n}-\mathbf{1}} - \mathbf{Q}^{\mathbf{n}}) \cdot \mathbf{Q}^{\mathbf{n}}}{\left\|\mathbf{Q}^{\mathbf{n}-\mathbf{1}} - \mathbf{Q}^{\mathbf{n}}\right\|^2}, \text{ where } \mathbf{Q}^{\mathbf{n}} = \mathbf{u}_{\mathrm{s}}^{\mathrm{n}}(\mathbf{x}) - \mathbf{u}_{\mathrm{p}}^{\mathrm{n}-1}(\mathbf{x})$$

* Y. Yu, F. F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations, CMAME, 340, 2018, pp. 905-931.

Local/Nonlocal Coupling*

- We can seek an optimal R (Robin coefficient) analytically for a simple problem



- Simplified Peridynamic Model
  - $\int_{H_x} c\left(\frac{\|\xi+\eta\|-\|\xi\|}{\|\xi\|}\frac{\xi+\eta}{\|\xi+\eta\|}\right) d V_{x'} = \mathbf{0},\ \mathbf{x}\in\Omega_p$
- Simplified Linear Elastic Model (ν = 1/3)
  - $\frac{3E}{2}\frac{\partial^2 \mathbf{u}_s}{\partial x^2} + \frac{3E}{8}\frac{\partial^2 \mathbf{u}_s}{\partial y^2} = \mathbf{0},\ \mathbf{x}\in\Omega_s$
- Boundary Conditions
  - Robin: $-\frac{3E}{2}\frac{\partial \mathbf{u}_s^n}{\partial \mathbf{x}} + R\mathbf{u}_s^n = -\frac{3E}{2}\frac{\partial \mathbf{u}_p^{n-1}}{\partial \mathbf{x}} + R\mathbf{u}_p^{n-1},\ \forall\ \mathbf{x}=L_1$
  - Dirichlet + Aitken: $\mathbf{u}_p^n(\mathbf{x}) = \tau^n \mathbf{u}_p^{n-1}(\mathbf{x}) + (\mathbf{1}-\tau^n)\mathbf{u}_s^n(\mathbf{x}),\ \ \forall\ \mathbf{x}\in L_2$

* Y. Yu, F. F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations, CMAME, 340, 2018, pp. 905-931.

Local/Nonlocal Coupling*

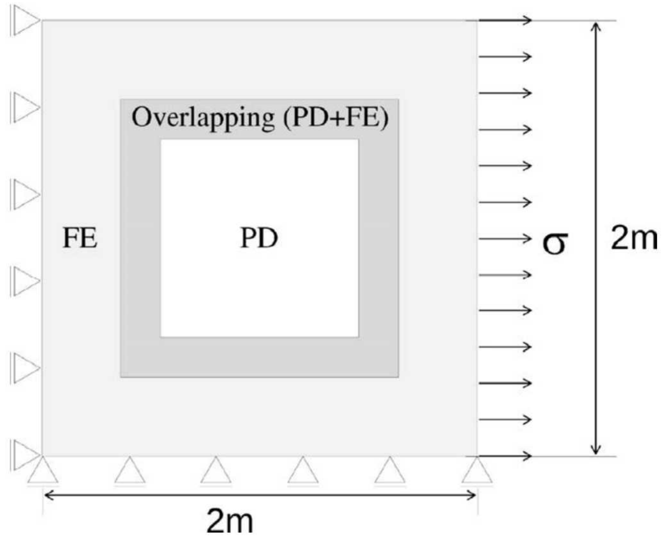
- Convergence analysis based on Fourier
  - $\mathbf{u}_\mathrm{s}(\mathrm{x},\mathrm{y}) = \sum_{\boldsymbol{\gamma}} (\hat{\mathrm{u}}_\mathrm{s})_{\boldsymbol{\gamma}}(\mathrm{x})\cos\left(\frac{\gamma\pi\mathrm{y}}{\mathrm{L}}\right)$, $\mathbf{u}_\mathrm{p}(\mathrm{x},\mathrm{y}) = \sum_{\boldsymbol{\gamma}} (\hat{\mathrm{u}}_\mathrm{p})_{\boldsymbol{\gamma}}(\mathrm{x})\cos\left(\frac{\gamma\pi\mathrm{y}}{\mathrm{L}}\right)$
- Define reduction factor in frequency space
  - $\rho_{\boldsymbol{\gamma}}^\mathrm{n} \coloneqq \frac{\left|(\hat{\mathrm{u}}_\mathbf{p}^\mathbf{n})_{\boldsymbol{\gamma}} - (\hat{\mathrm{u}}_\mathrm{p})_{\boldsymbol{\gamma}}\right|}{\left|(\hat{\mathrm{u}}_\mathbf{p}^\mathbf{n-1})_{\boldsymbol{\gamma}} - (\hat{\mathrm{u}}_\mathrm{p})_{\boldsymbol{\gamma}}\right|}$
- The reduction factor can be determined analytically as a function of R, τ^n:

$$
\begin{aligned}
\rho_\gamma^n(R,\tau^n) &= \left| \frac{(\tilde{u}_p^n)_\gamma \left(e^{\frac{\pi\tilde{\gamma}x}{2L}} - e^{\frac{-\pi\tilde{\gamma}x}{2L}}\right)}{(\tilde{u}_p^{n-1})_\gamma \left(e^{\frac{\pi\tilde{\gamma}x}{2L}} - e^{\frac{-\pi\tilde{\gamma}x}{2L}}\right)} \right| = \left| \frac{(\tilde{u}_p^n)_\gamma}{(\tilde{u}_p^{n-1})_\gamma} \right| \\
&= \left| \tau^n + (1-\tau^n) \frac{\left(-\frac{3E\pi\tilde{\gamma}}{4L}\left(e^{\frac{\pi\tilde{\gamma}L_1}{2L}} + e^{\frac{-\pi\tilde{\gamma}L_1}{2L}}\right) + R\left(e^{\frac{\pi\tilde{\gamma}L_1}{2L}} - e^{\frac{-\pi\tilde{\gamma}L_1}{2L}}\right)\right)\left(e^{\frac{\pi\gamma L_2}{2L}} - e^{\frac{-\pi\gamma L_2}{2L}}\right)}{\left(-\frac{3E\pi\gamma}{4L}\left(e^{\frac{\pi\gamma L_1}{2L}} + e^{\frac{-\pi\gamma L_1}{2L}}\right) + R\left(e^{\frac{\pi\gamma L_1}{2L}} - e^{\frac{-\pi\gamma L_1}{2L}}\right)\right)\left(e^{\frac{\pi\tilde{\gamma}L_2}{2L}} - e^{\frac{-\pi\tilde{\gamma}L_2}{2L}}\right)} \right|
\end{aligned}
$$

* Y. Yu, F. F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations, CMAME, 340, 2018, pp. 905-931.

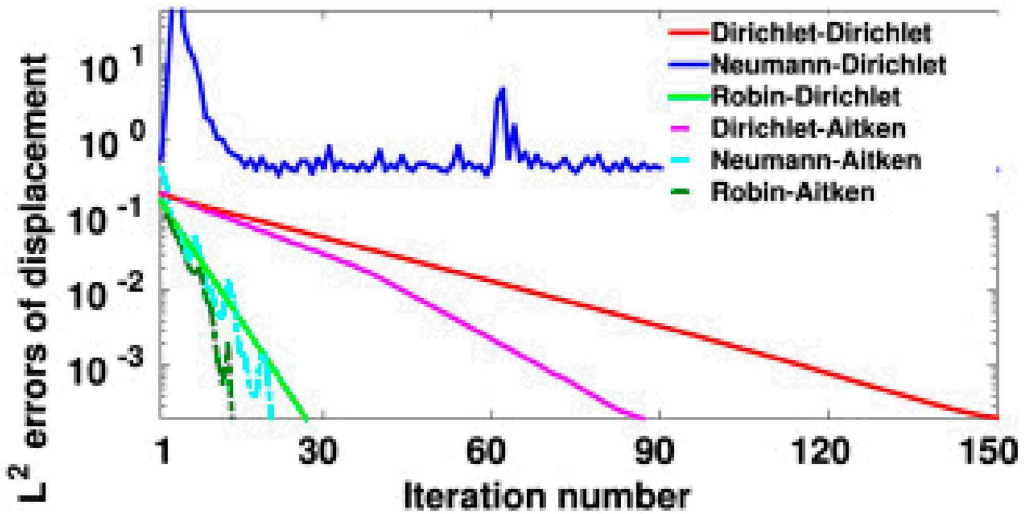
Local/Nonlocal Coupling*

- Test problem: Plate under uniaxial tension
- Manufactured solution satisfies both local and nonlocal



- $\mathbf{u}_s(x,y) = \begin{bmatrix} \frac{0.8(1-\upsilon)(1+\upsilon)}{E}(x+1) \\ -\frac{0.8\upsilon(1+\upsilon)}{E}(y+1) \end{bmatrix}$

- Convergence with optimal R, τ^n:
  - Optimal Robin–Aitken (16 steps)
  - Optimal Robin–Dirichlet (35 steps)
  - Neumann–Aitken (39 steps)
  - Dirichlet–Aitken (94 steps)
  - Dirichlet–Dirichlet (161 steps)
  - Neumann–Dirichlet (divergent).



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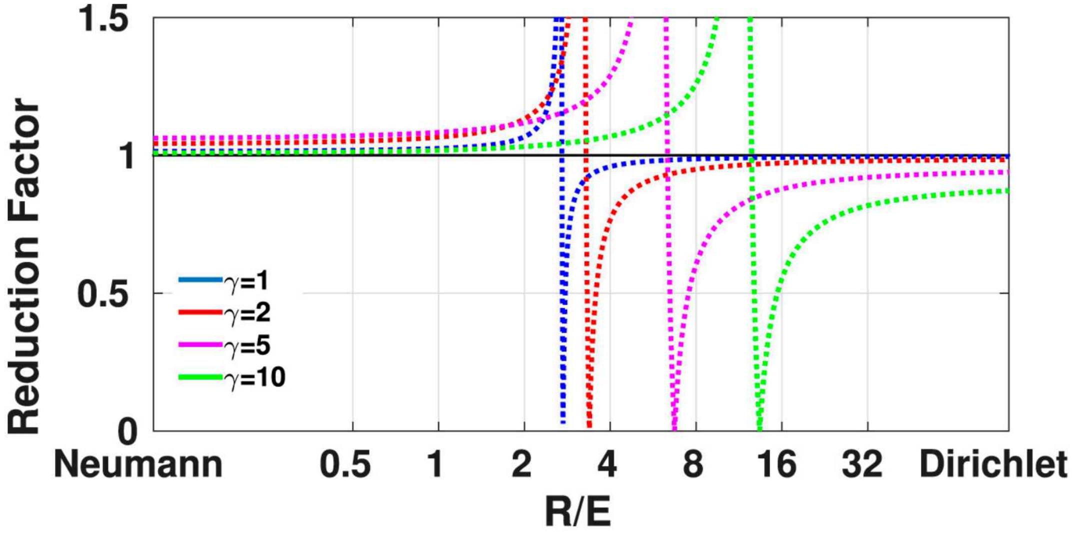
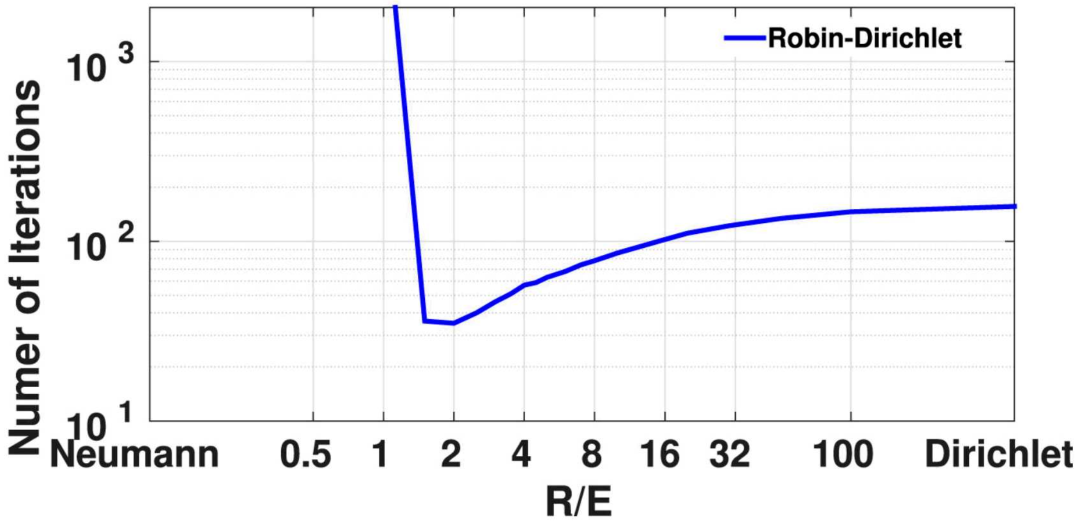
Local/Nonlocal Coupling*

- Test problem: Plate under uniaxial tension



Reduction factor for various frequencies for 1D analysis



 # Iterations for convergence for 2D plate under uniaxial tension

* Y. Yu, F. F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations, CMAME, 340, 2018, pp. 905-931.

Local/Nonlocal Coupling*

- Example with fracture in peridynamic domain

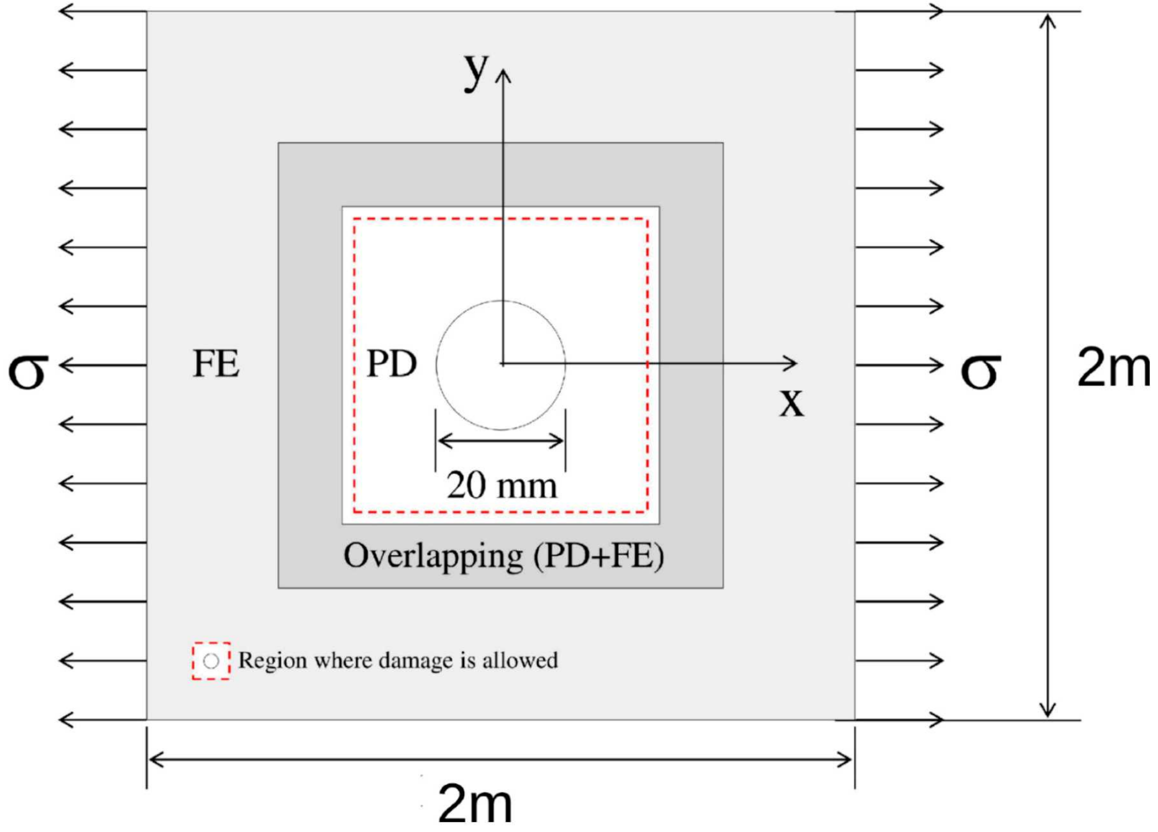
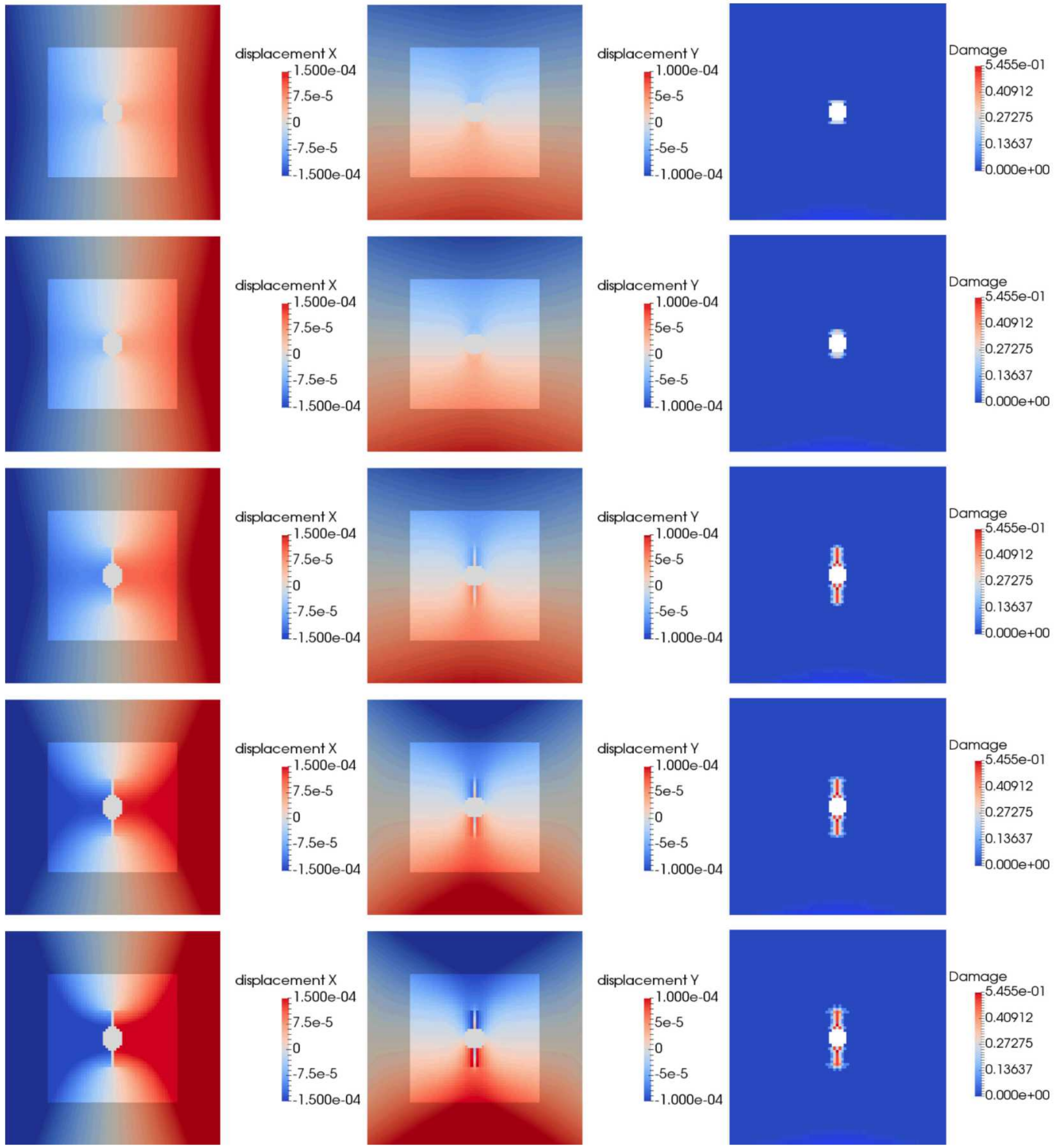


Plate with hole under uniaxial tension



x-displacement y-displacement damage

* Y. Yu, F. F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations, CMAME, 340, 2018, pp. 905-931.

Conclusions

Today, we discussed:

- Historical and mathematical origins of Alternating Schwarz
- Some convergence analysis
- Applications to multiscale and multi-model coupling:
  - Atomistic-to-continuum
  - Local/Nonlocal coupling