

Numerical Solution of Vector-Valued Phase Field Models

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DIMO 2013 – Diffuse Interface Models

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Synopsis

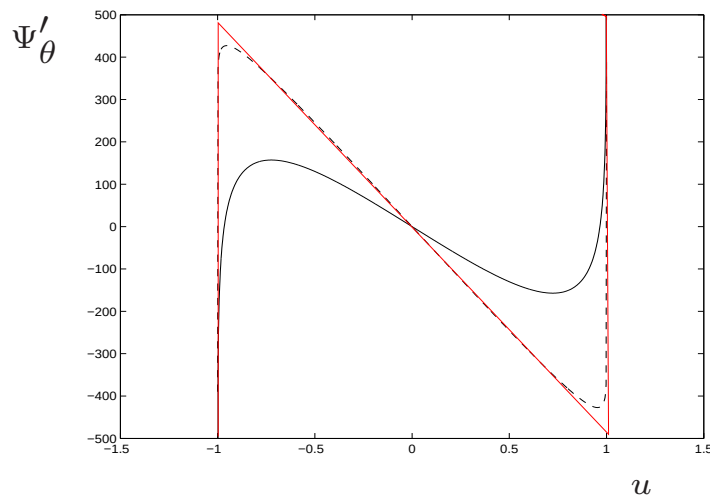
- phase transition and phase separation
- vector-valued Allen-Cahn equations (Bronsard & Reitich 93, Garcke et al. 98, 99a, 99b)
 - robust formulation of discrete spatial problems (logarithmic $\rightsquigarrow$ obstacle potential)
 - polygonal Gauß-Seidel relaxation (Kh. & Krause 03, 06)
 - truncated non-smooth Newton multigrid (TNNMG) (Gräser & Kh. 09, Gräser 11)
 - numerical experiments
- vector-valued Cahn-Hilliard equations (Blowey et al. 96, Barret & Blowey 96, 97, Gräser, Kh. & Sack 13)
 - robust formulation of discrete spatial problems
 - truncated Schur Newton methods (Gräser & Kh. 06, 09, Gräser 08, 11)
 - numerical experiments

Ginzburg-Landau Approach to Phase Transition/Separation

Ginzburg-Landau free energy: $\mathcal{E}(u) = \int_{\Omega} \varepsilon |\nabla u|^2 + \frac{1}{\varepsilon} \Psi_{\theta}(u) \, dx$

order parameter (phase field): $u \in [-1, +1]$

diffuse interface: $\Gamma_{\varepsilon} = \{x \in \Omega \mid u(x) \in (u_a, u_b)\}$, binodal values $u_a, u_b \in [-1, 1]$



logarithmic free energy: (Giacomin & Lebowitz 98)

$$\Psi_{\theta}(u) = \frac{1}{2}\theta((1-u)\ln(\frac{1-u}{2}) + (1+u)\ln(\frac{1+u}{2})) + \frac{1}{2}\theta_c(1-u^2)$$

temperature θ , critical temperature θ_c

deep quench limit: $\theta \rightarrow 0 \Rightarrow \Psi_{\theta} \rightarrow \Psi_0$

Phase Field Models

isothermal case: $\theta = \text{const.}$

phase transition: Allen-Cahn equation (non-conserving)

$$\varepsilon u_t = -\frac{d}{du}\mathcal{E}(u) = \varepsilon \Delta u - \frac{1}{\varepsilon} \Psi'_\theta(u) \quad (\text{Cahn 60, Allen \& Cahn 77})$$

phase separation: Cahn-Hilliard equations (conserving)

$$\varepsilon u_t = \Delta w, \quad w = \frac{d}{du}\mathcal{E}(u) = -\varepsilon \Delta u + \frac{1}{\varepsilon} \Psi'_\theta(u) \quad (\text{Cahn \& Hilliard 58})$$

Lyapunov functional: $\frac{d}{dt}\mathcal{E}(u(t)) \leq 0$

deep quench limit $\theta = 0$: variational inequalities

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deep quench limit $\theta = 0$: variational inequalities

robustness of numerical solvers for $\theta \rightarrow 0$ (Kh. & Krause 03, 06, Gräser & Kh. 09, Gräser 11)

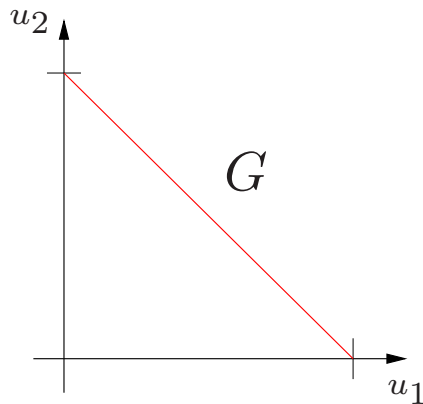
N Phases

concentrations: $u_1, \dots, u_N$

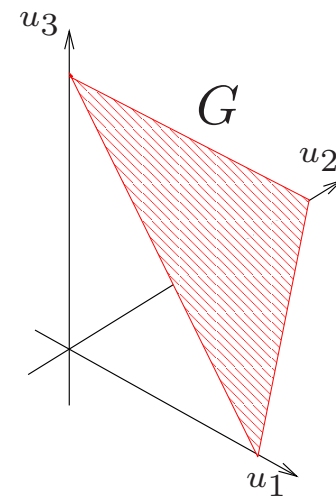
vector-valued phase field: $u = (u_1, \dots, u_N) \in \mathbb{R}^N$

Gibbs simplex: $u(x, t) \in G = \{v \in \mathbb{R}^N \mid 0 \leq v_i, \sum_{i=1}^N v_i = 1\}$ (closed, convex)

N=2:



N=3:



Ginzburg-Landau Free Energy

$$\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} \sum_{i=1}^N |\nabla u_i|^2 + \frac{1}{\varepsilon} \Psi_{\theta}(u) \, dx, \quad \varepsilon > 0$$

multi-well potential: $\Psi_{\theta}(u) = \Phi_{\theta}(u) + \chi_{H_1}(u) + \theta_c \frac{N}{2} C u \cdot u$

$$\Phi_{\theta}(u) = \begin{cases} \sum_{i=1}^N \theta u_i \ln(u_i) + \chi_{[0,\infty)}(u_i), & \theta > 0 \\ \chi_{[0,\infty)}(u_i), & \theta = 0 \end{cases}$$

$$H_1 = \{v \in \mathbb{R}^N \mid \sum_{i=1}^N v_i = 1\}$$

critical temperature: $\theta_c = 1$

symmetric interaction matrix: $C = (1 - \delta_{ij})_{i,j=1}^N$

Vector-Valued Allen-Cahn Equations

projected L^2 -gradient flow of $\mathcal{E}$:

$$\varepsilon u_t = \varepsilon \Delta u - \frac{1}{\varepsilon} P \Psi'_\theta(u), \quad P = I - \frac{1}{N} \mathbf{1} \mathbf{1}^\top \in \mathbb{R}^{N \times N}, \quad \theta > 0$$

parabolic variational inequality (Bronsard & Reitich 93, Garcke et al. 98, 99a, 99b):

$$\begin{aligned} u(t) \in \mathcal{G} : \quad & \varepsilon(u_t, v - u) + \varepsilon(\nabla u, \nabla(v - u)) \\ & + \frac{1}{\varepsilon} (\phi_\theta(v) - \phi_\theta(u)) - N \frac{1}{\varepsilon} (u, v - u) \geq 0 \quad \forall v \in \mathcal{G} \end{aligned} \quad \theta \geq 0$$

proper convex, lower semi-continuous functional: $\phi_\theta(v) = \int_\Omega \Phi_\theta(v(x)) \, dx$

Gibbs constraints: $\mathcal{G} = \left\{ v \in (H^1(\Omega))^N \mid v(x) \in G \text{ a.e. in } \Omega \right\}$

Discretization

implicit Euler discretization: stepsize τ

linear finite elements $\mathcal{S}_j^N$:

triangulation $\mathcal{T}_j$, meshsize $h_j = \mathcal{O}(2^{-j})$, nodes $\mathcal{N}_j$, nodal basis $\lambda_p^{(j)}$ of $\mathcal{S}_j$

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discrete spatial problems:

$$u_j \in \mathcal{G}_j : \quad (u_j, v - u_j) + \tau(\nabla u_j, \nabla(v - u_j)) \\ + \frac{\tau}{\varepsilon^2} (\phi_{\theta,j}(v) - \phi_{\theta,j}(u)) - N \frac{\tau}{\varepsilon^2} (u_j, v - u_j) \geq (u_j^{\text{old}}, v - u_j) \quad \forall v \in \mathcal{G}_j$$

quadrature rule (lumping): $\phi_{\theta,j} = \int_{\Omega} I_{\mathcal{S}_j^N} \Phi_{\theta}(v) \, dx$

discrete Gibbs constraints: $\mathcal{G}_j = \{v \in \mathcal{S}_j^N \mid v(p) \in G \, \forall p \in \mathcal{N}_j\}$

Discretization

implicit Euler discretization: stepsize $\tau < \frac{\varepsilon^2}{N}$

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Convex Minimization

variational inequality:

$$u_j \in \mathcal{G}_j : \quad a(u_j, v - u_j) + \frac{\tau}{\varepsilon^2} (\phi_j(v) - \phi_j(u)) \geq \ell(v - u_j) \quad \forall v \in \mathcal{G}_j$$

bilinear form: $a(v, w) = (1 - N \frac{\tau}{\varepsilon^2})(v, w) + \tau(\nabla v, \nabla w)$ $(H^1(\Omega))^N$ -elliptic

linear functional: $\ell(v) = (u_j^{\text{old}}, v)$

equivalent reformulation:

$$u_j \in \mathcal{G}_j : \quad \mathcal{J}(u_j) \leq \mathcal{J}(v) \quad \forall v \in \mathcal{G}_j$$

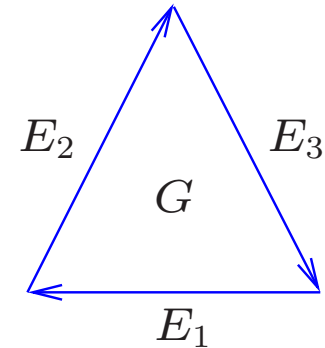
strictly convex energy: $\mathcal{J}(v) = \frac{1}{2}a(v, v) + \frac{\tau}{\varepsilon^2}\phi_j(v) - \ell(v)$

Polygonal Gauß-Seidel Relaxation (Kh. & Krause 03)

descent directions: $\lambda_p^{(j)} E_m$, $p \in \mathcal{N}_j$, $m = 1, \dots, M$

edge vectors of G :

$$E_1, \dots, E_M \in \mathbb{R}^N, \quad M := \frac{N(N-1)}{2} = \mathcal{O}(N^2)$$

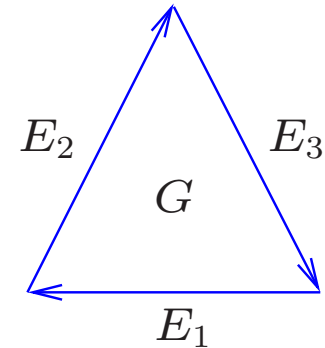


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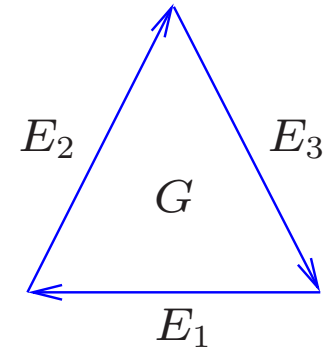
successive minimization of $\mathcal{J} + \chi_{\mathcal{G}_j}$
on 1-D subspaces $\text{span}\{\lambda_p^{(j)} E_m\}$, $p \in \mathcal{N}_j$, $m = 1, \dots, M$

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complexity: $\mathcal{O}(N^2 n_j)$

global convergence (Kh., Krause & Ziegler 06)

exponentially deteriorating convergence speed: $\rho_j = 1 - \mathcal{O}(2^{-j})$

Fast Algebraic Solvers

- **monotone multigrid (MMG)** (Kh & Krause 03, 06)

multilevel version of Gauß-Seidel relaxation

robust global convergence for $\theta \geq 0$ with asymptotic multigrid convergence rates

- **primal-dual active set strategy** (Blank, Garcke, Sarbu & Styles 11)

obstacle potential, local convergence

- **truncated non-smooth Newton multigrid (TNNMG)** (Gräser & Kh 09, Gräser 11, 13, ...)

motivated by a non-smooth Newton approach

robust global convergence for $\theta \geq 0$ with asymptotic multigrid convergence rates

faster and simpler to implement than MMG

Truncated Non-Smooth Newton Multigrid (TNNMG)

convex minimization:

$$u \in \mathbb{R}^n : \quad J(u) \leq J(v) \quad \forall v \in \mathbb{R}^n, \quad J(v) = \frac{1}{2}Av \cdot v - b \cdot v + \Psi(v)$$

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reformulation in terms of polygonal Gauß-Seidel correction:

$$u^{\nu+1} = u^{\nu} + F(u^{\nu})$$

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non-smooth Newton iteration:

$$-\partial F(u^{\nu})(u^{\nu+1} - u^{\nu}) = F(u^{\nu})$$

Generalized Linearization ∂F (Gräser 11)

Gauß-Seidel correction: $F(u) = (D + \partial\Psi)^{-1}(b - (R + L)u - LF(u)), \quad A = L + D + R$

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Clarke's generalized derivative:

$$(D + \partial\Psi)^{-1}(w) = (f_i(w_i))_{i=1}^n, \quad f_i(w_i) = (A_{ii} \cdot + \partial\Psi_i(\cdot))^{-1}(w_i)$$

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enforcing of chain rule: non-smooth Newton Linearization

$$u^{\nu+1/2} = u^{\nu} + F(u^{\nu}), \quad u^{\nu+1} = u^{\nu+1/2} - J''_{\mathcal{I}(u^{\nu+1/2})}(u^{\nu+1/2}) + J'_{\mathcal{I}(u^{\nu+1/2})}(u^{\nu+1/2})$$

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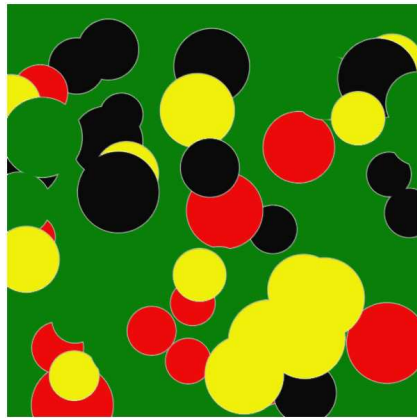
TNNMG: fine grid smoothing + truncated multigrid step + projection + line search

Numerical Experiments

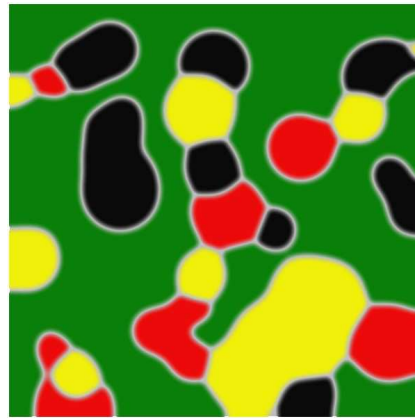
parameter: $\theta = 0$, $N = 4$, $\varepsilon = 0.04$, $\theta_c = 1$

discretization: implicit Euler scheme, $\tau = \frac{3}{4}\varepsilon^2/N$, $j = 9$: $h_j = 1/256 \approx \varepsilon/10$

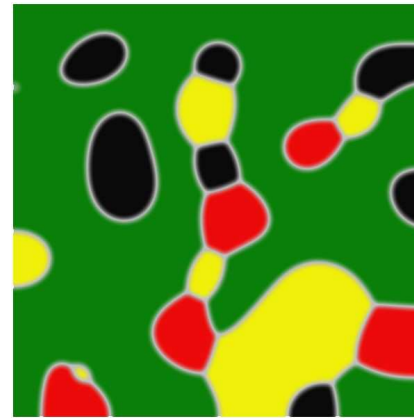
evolution:



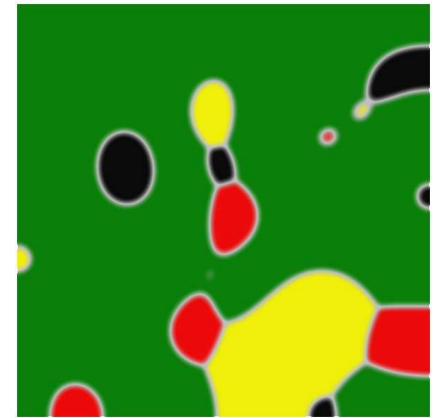
$t = 0$



$t = 10\tau$



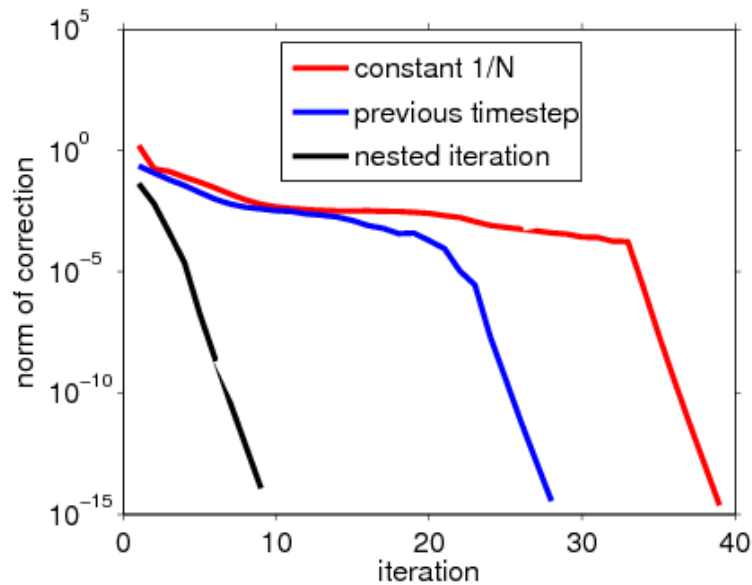
$t = 50\tau$



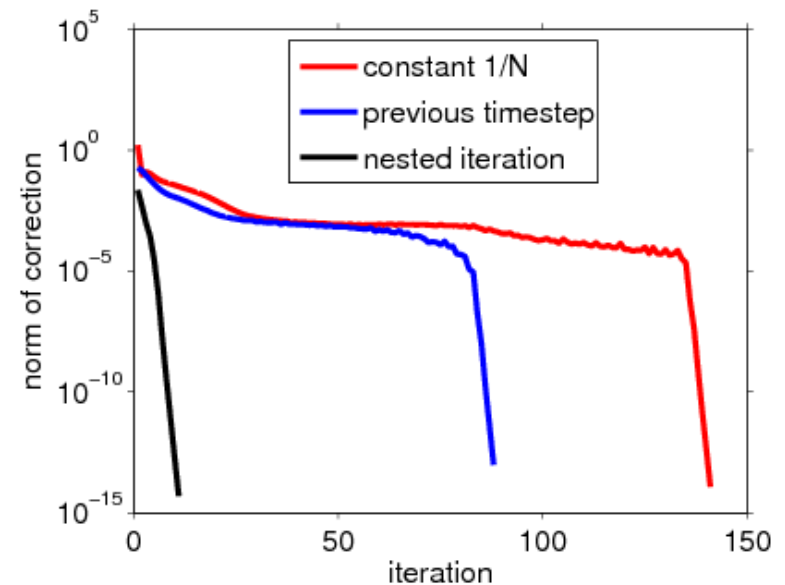
$t = 100\tau$

Iteration History (First Spatial Problem)

error over number of iteration steps for $V(1, 1, 0)$ cycle:



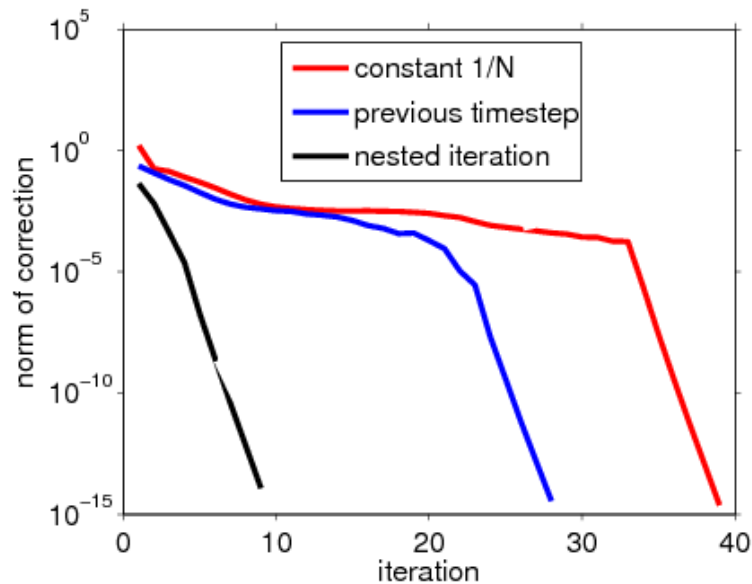
$\# \text{nodes} = 263\,169$



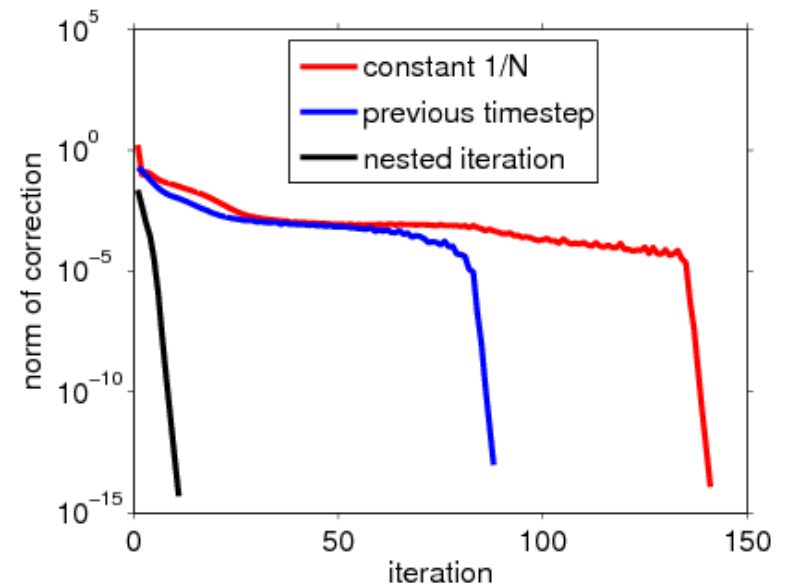
$\# \text{nodes} = 1\,050\,625$

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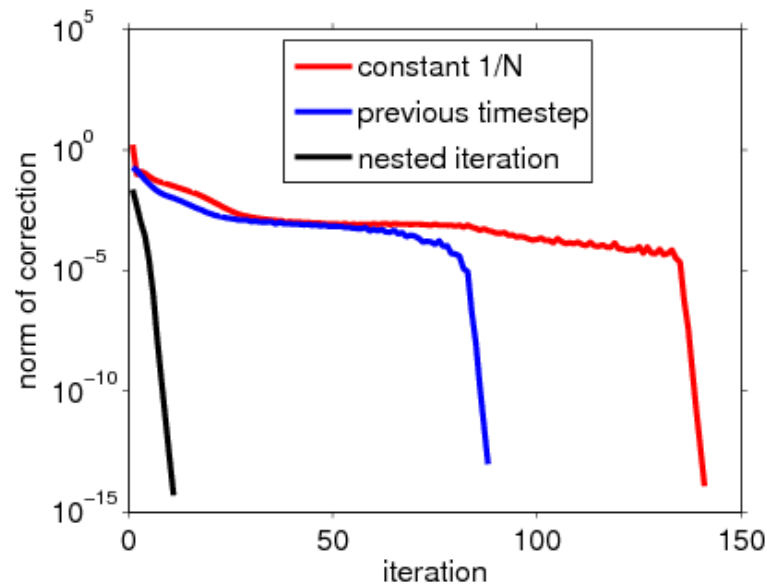


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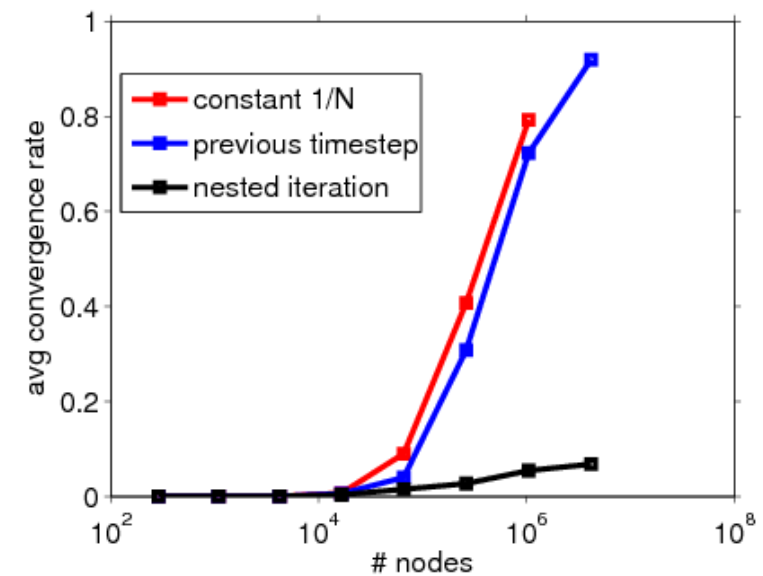
global convergence and local multigrid convergence speed

Local Mesh Independence of Convergence Speed

mesh-dependent global convergence and mesh-independence by nested iteration:



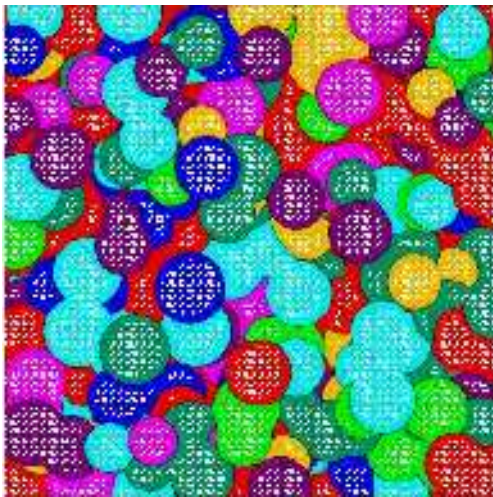
#nodes = 1 050 625



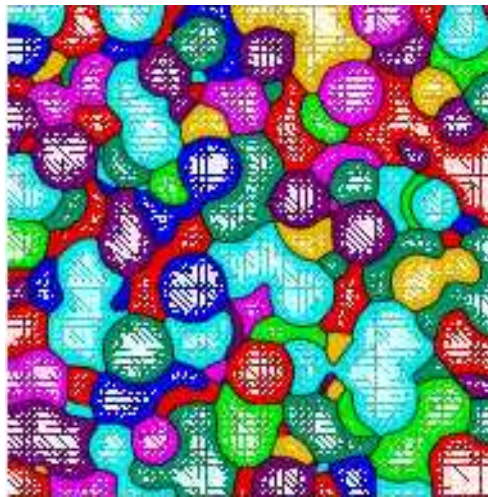
More Phases

parameter: $\theta = 0$, $N = 8$, $\varepsilon = 0.04$, $\theta_c = 1$

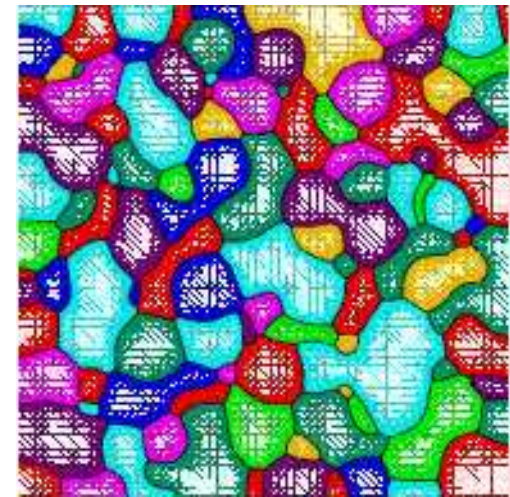
evolution:



$t = 0$



$t = 10\tau$

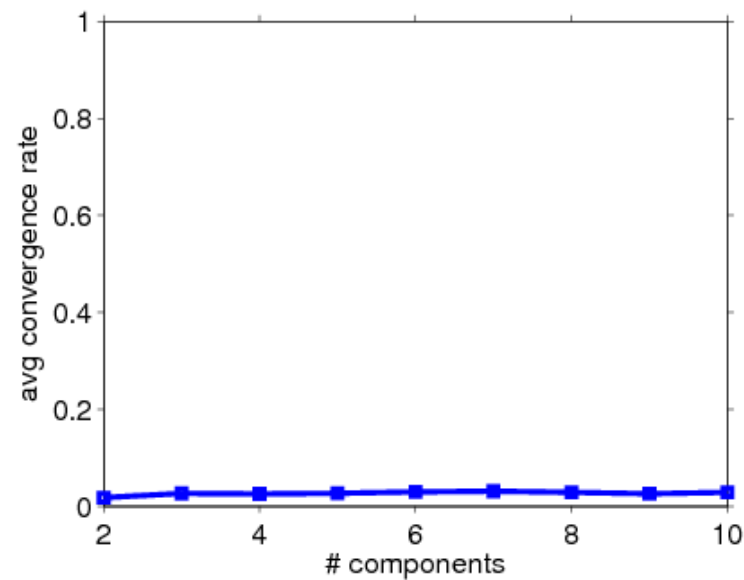


$t = 40\tau$

Robustness of Convergence Speed w.r.t. N

initial value: nested iteration #nodes: 263 169

averaged convergence rate over number of components N :



Vector-Valued Cahn-Hilliard Equations

$$u_t = L\Delta w, \quad w = -\varepsilon^2 \Delta u + P\Psi'_\theta(u), \quad \theta > 0$$

$$L \in \mathbb{R}^{N \times N}, \quad \text{s.p.s.-d.}, \quad \ker L = \text{span} \{ \mathbf{1} \}$$

weak formulation: Find $(u(t), w) \in \mathcal{G} \times H^1(\Omega)^N$:

$$\begin{aligned} \varepsilon^2(\nabla u, \nabla v) + (P\Psi'_\theta(u), v) - (w, v) &= 0 \quad \forall v \in H^1(\Omega)^N \\ (u_t, v) + (L\nabla w, \nabla v) &= 0 \quad \forall v \in H^1(\Omega)^N \end{aligned} \quad \theta > 0$$

existence and uniqueness: Elliott & Luckhaus 91

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Remark: $(I - P)u = \frac{1}{N}\mathbf{1}, \quad (I - P)w = 0$

Discretization

semi-implicit Euler scheme, linear finite elements $\mathcal{S}_j^N$

spatial problems: Find $(u_j, w_j) \in \mathcal{G}_j \times \mathcal{S}_j^N$:

$$\begin{aligned} (BB) \quad \varepsilon^2(\nabla u_j, \nabla v) + (P\Phi'_j(u_j), v) - (w_j, v) &= (Nu^{\text{old}} - \mathbf{1}, v) & \forall v \in \mathcal{S}_j^N \\ (u_j, v) + \tau(L\nabla w, \nabla v) &= (u^{\text{old}}, v) & \forall v \in \mathcal{S}_j^N \end{aligned}$$

existence, uniqueness, convergence: Blowey, Copetti & Elliott 96

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existence, uniqueness, convergence: Blowey, Copetti & Elliott 96

formulation not robust for $\theta \rightarrow 0$

Discretization

semi-implicit Euler scheme, linear finite elements $\mathcal{S}_j^N$

spatial problems: Find $(u_j, w_j) \in \mathcal{G}_j \times \mathcal{S}_j^N$:

$$\begin{aligned} (BB) \quad \varepsilon^2(\nabla u_j, \nabla v) + (\mathbf{P}\Phi'_j(u_j), v) - (w_j, v) &= (Nu^{\text{old}} - \mathbf{1}, v) & \forall v \in \mathcal{S}_j^N \\ (u_j, v) + \tau(L\nabla w, \nabla v) &= (u^{\text{old}}, v) & \forall v \in \mathcal{S}_j^N \end{aligned}$$

existence, uniqueness, convergence: Blowey, Copetti & Elliott 96

formulation not robust for $\theta \rightarrow 0$

linear constraints (polygonal Gauß - Seidel)

Robust Reformulation: $w_j \rightsquigarrow Pw_j$

reduced test space: $\mathcal{S}_{j,0}^N = \{v \in \mathcal{S}_j^N \mid \sum v_i = 0\}$

$$\begin{aligned}\varepsilon^2(\nabla u_j, \nabla v) + (\Phi'_j(u_j), v) - (w_j, v) &= (Nu^{\text{old}} - \mathbf{1}, v) & \forall v \in \mathcal{S}_{j,0}^N \\ (u_j, v) + \tau(L\nabla w_j, \nabla v) &= (u_j^{\text{old}}, v) & \forall v \in \mathcal{S}_{j,0}^N\end{aligned}$$

robust formulation for $\theta \geq 0$: Find $(u_j, w_j) \in \mathcal{S}_{j,1}^N \times \mathcal{S}_{j,0}^N$:

$$\begin{aligned}\varepsilon^2(\nabla u_j, \nabla(v - u_j)) + \phi_j(v) - \phi_j(u_j) \\ -(w_j, v - u_j) &\geq (Nu_j^{\text{old}}, v - u_j) & \forall v \in \mathcal{S}_{j,1}^N \\ (u_j, v) + \tau(L\nabla w_j, \nabla v) &= (u_j^{\text{old}}, v) & \forall v \in \mathcal{S}_{j,0}^N\end{aligned}$$

Robust Reformulation without Linear Constraints: $w_j \rightsquigarrow w_j + \eta_j \mathbf{1}$

Lagrange multiplier η_j : $(u, \mathbf{1}v) = (u^{\text{old}}, \mathbf{1}v) = (1, v)$

unconstrained spatial problem for all $\theta \geq 0$: Find $(u_j, w_j) \in \mathcal{S}_j^N \times \mathcal{S}_j^N$:

$$\varepsilon^2(\nabla u_j, \nabla(v - u_j)) + \phi_j(v) - \phi_j(u_j)$$

$$(GKS) \quad -(w_j, v - u_j) \geq (Nu_j^{\text{old}}, v - u_j) \quad \forall v \in \mathcal{S}_j^N$$

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Theorem: (Gräser, Kh. & Sack 12)

non-degeneracy + sufficiently fine mesh $\Rightarrow$ existence and uniqueness of (u, w) .

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Theorem: $\theta > 0$: (u, w) solves (BB) $\iff (u, Pw + \eta \mathbf{1})$ solves (GKS)

Non-Smooth Saddle-Point Problem

$$\begin{pmatrix} F & B^T \\ B & -C \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} \ni \begin{pmatrix} f \\ g \end{pmatrix}$$

$$F = A + \partial\Phi, \quad A \in \mathbb{R}^{n,n} \text{ s.p.d.}, \quad B \in \mathbb{R}^{m,n}, \quad C \in \mathbb{R}^{m,m} \text{ s.p. s.-d.}$$

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basic observation: (Gräser & Kh. 09)

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convex potential: $H = \nabla \mathcal{J}$

unconstrained (!) convex minimization: $w \in \mathbb{R}^n$: $\mathcal{J}(w) \leq \mathcal{J}(v) \quad \forall v \in \mathbb{R}^n$

Nonsmooth Schur Newton Iteration (Gräser & Kh. 06, 09, Gräser 08, 11)

basic properties:

- gradient-related descent method (global convergence by damping!)
- preconditioned Uzawa iteration
- extension and globalization of primal-dual active sets
- first formulation in function space: Hinze & Vierling 2012

numerical realization of each iteration step:

- vector-valued Allen-Cahn-type problem (unilateral box constraints!): TNNMG
- linear saddle point problem: multigrid-preconditioned GMRES

Convergence Properties

Theorem: Global convergence.

expected numerical convergence properties:

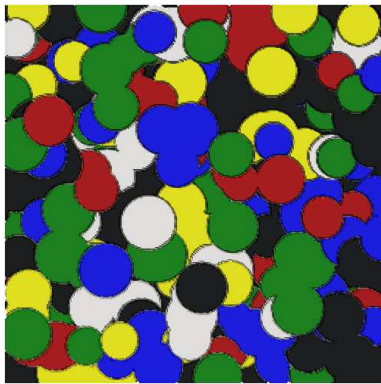
- superlinear convergence
- no damping and fast convergence for “good” initial iterates
- nested iteration provides “good” initial iterates
- nested iteration provides mesh-independent convergence
- logarithmic potential: robust convergence for varying temperature $T \in [0, T_c]$

Numerical Experiments

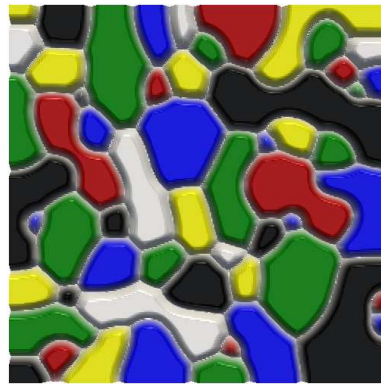
parameter: $L = I - \frac{1}{N}\mathbf{1}\mathbf{1}^\top = P$, $\theta = 0.1$, $N = 6$, $\varepsilon^2 = 0.005$, $\theta_c = 1$

discretization: semi-implicit Euler scheme, $\tau = \varepsilon^2/5$, $j = 8$: $h_j = 2^{-j} \approx \varepsilon/9$

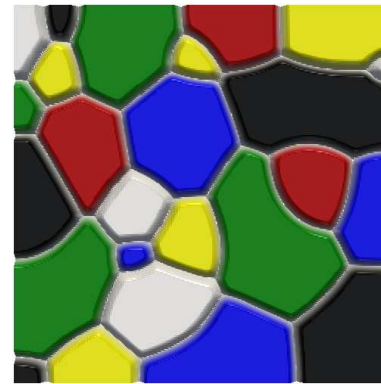
evolution:



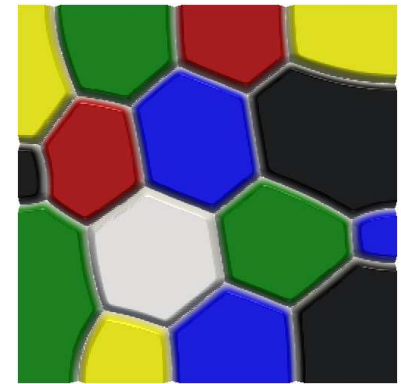
$t = 0$



$t = 20\tau$



$t = 200\tau$



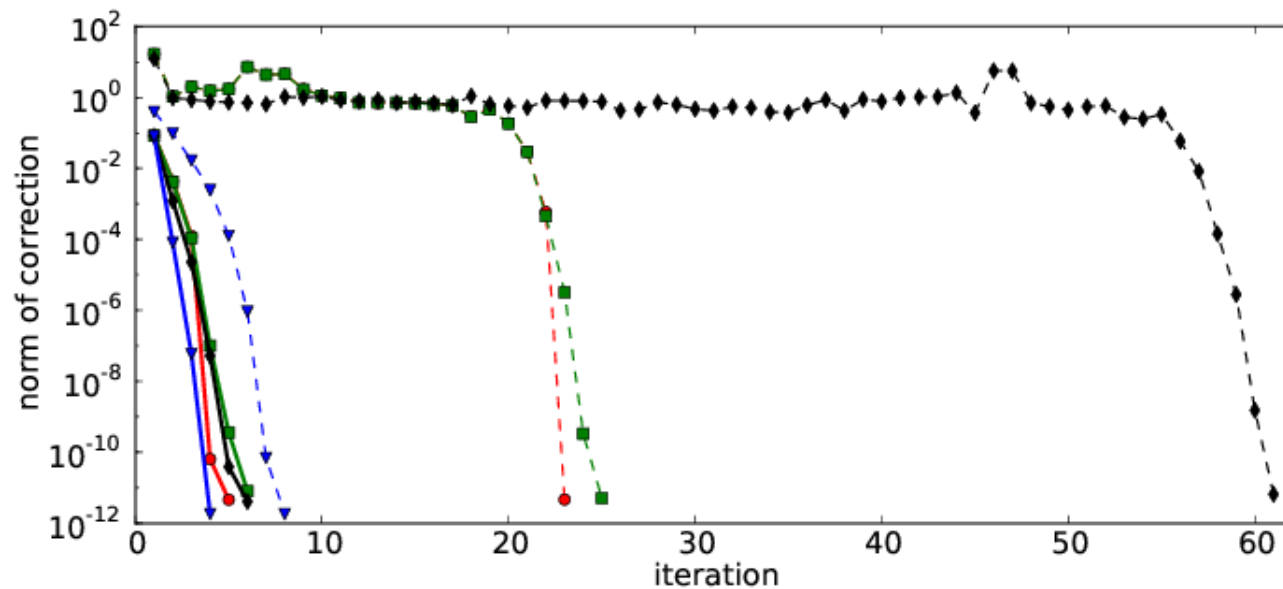
$t = 1000\tau$

Superlinear Convergence and Nested Iteration

algebraic error over number of iterations:

“bad” (---) and “good” (—) initial iterates

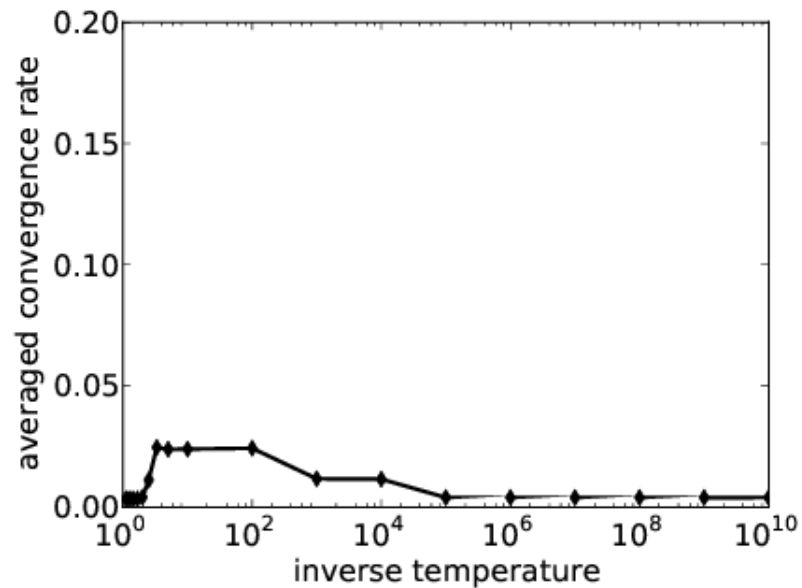
various temperatures $\theta = 0.0, 0.001, 0.1, 0.5$



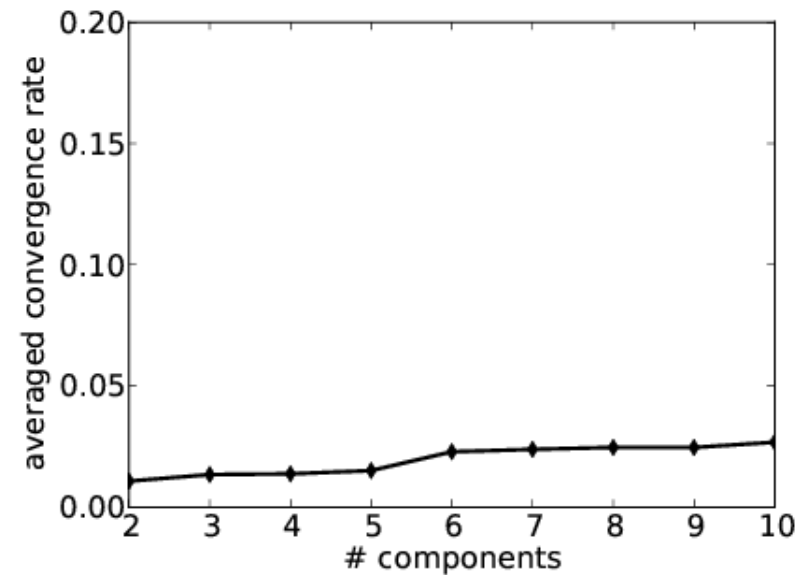
Robustness w.r.t. Temperature θ and Number of Phases N

averaged convergence rate over

inverse temperature θ

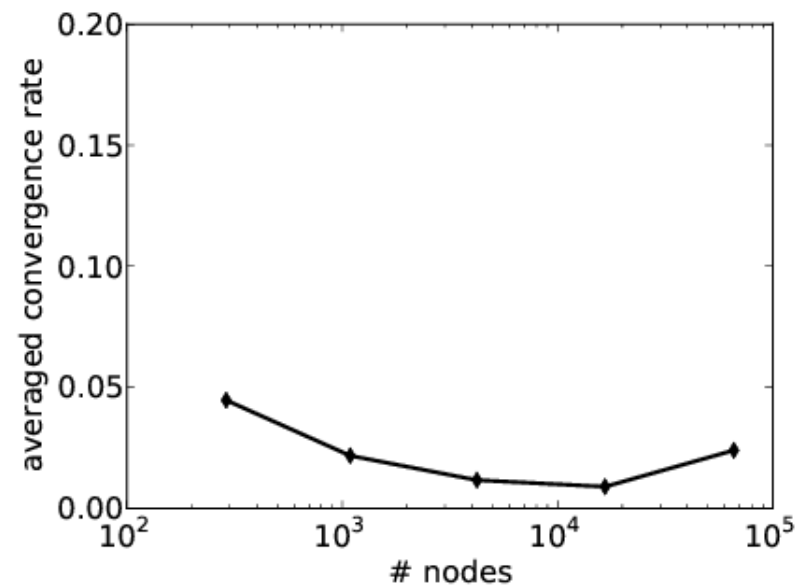


number of Phases N



Mesh-Dependence

averaged convergence rate over number of nodes ($N = 6$, $\theta = 0.1$):



Fast Solvers for Vector-Valued Phase Field Equations

vector-valued Allen-Cahn equations

- polygonal Gauß-Seidel relaxation (Kh. & Krause 03, 06)
- truncated non-smooth Newton multigrid (TNNMG) (Gräser & Kh. 09, Gräser 11)

vector-valued Cahn-Hilliard equations (Gräser, Kh. & Sack 13)

- fast solver for Allen-Cahn-type problem + linear saddle point solver
- truncated Schur Newton methods (Gräser & Kh. 06, 09, Gräser 08, 11)

Nonlinear Schur Complement

$$\begin{pmatrix} F & B^T \\ B & -C \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} \ni \begin{pmatrix} f \\ g \end{pmatrix}$$

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Proposition

Let $\varphi^* : \mathbb{R}^n \mapsto \mathbb{R}$ denote the polar functional of φ with $F = \partial\varphi$

- $\mathcal{J}(\lambda) = \varphi^*(f - B^T\lambda) + \frac{1}{2}(C\lambda, \lambda) + (g, \lambda)$ is Fréchet-differentiable
- $H = \nabla \mathcal{J}$
- $H(\lambda) = 0$ is equivalent to **unconstrained (!) convex minimization**

$$\lambda \in \mathbb{R}^n : \quad \mathcal{J}(\lambda) \leq \mathcal{J}(v) \quad \forall v \in \mathbb{R}^n$$

Gradient-Related Descent Methods

$$\lambda^{\nu+1} = \lambda^{\nu} + \rho_{\nu} d_{\nu} , \quad d_{\nu} = -S_{\nu}^{-1} \nabla \mathcal{J}(\lambda^{\nu}) , \quad S_{\nu} \text{ s.p.d.}$$

Assumption on d_{ν} : $c\|v\|^2 \leq (S_{\nu}v, v) \leq C\|v\|^2 \quad \forall \nu \in \mathbb{N}$

Assumption on ρ_{ν} : $\mathcal{J}(\lambda^{\nu} + \rho_{\nu} d_{\nu}) \leq \mathcal{J}(\lambda^{\nu}) - c(\nabla \mathcal{J}(\lambda^{\nu}), d_{\nu})^2 / \|d_{\nu}\|^2$

Theorem: (... , Ortega & Rheinboldt 70, Nocedal 92, Powell 98, Deuffhard 04, ...)

The iteration is globally convergent.

Damping Strategies

classical Armijo damping: two parameters, expensive evaluation of $\mathcal{J}$

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inexact damping: approximate the solution of $(H(\lambda^\nu + \rho d_\nu), d_\nu) = 0$ by bisection

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numerical experience: usually 1 step, but up to 8 steps in exceptional cases

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monotonicity test: (Gräser & Kh. 09, Gräser 10)

no damping necessary, if $\|d_\nu\| \leq \sigma \|d_{\nu-1}\|, \quad \sigma < 1$

Inexact Evaluation of S_ν^{-1}

Proposition:

Let $\tilde{d}_\nu \approx d_\nu = -S_\nu^{-1} \nabla \mathcal{J}(\lambda^\nu)$.

Then the accuracy conditions

$$\|d_\nu - \tilde{d}_\nu\| \leq \frac{1}{\nu} \|d_\nu\|, \quad (H(\lambda^\nu), \tilde{d}_\nu) < 0 \quad \forall \nu \in \mathbb{N}$$

preserve convergence.

Selection of S_ν : Nonsmooth Schur Newton Methods

gradient-related descent method:

$$\lambda^{\nu+1} = \lambda^\nu - \rho_\nu S_\nu^{-1} H(\lambda^\nu)$$

$$H(\lambda^\nu) = -Bu^{\nu+1} + C\lambda^\nu + g, \quad u^{\nu+1} = F^{-1}(f - B^T \lambda^\nu)$$

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Selection of $\delta(F^{-1})(F(u^{\nu+1}))$: Truncated Derivatives

postulating the chain rule: $\delta(F^{-1})(F(u^{\nu+1})) := \left(\hat{F}'(u^{\nu+1})\right)^+$

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characteristic function $\Phi = \chi_{[-1,1]}$: (box constraints)

$$F = A + \partial\chi_{[-1,1]}: \quad \delta(F^{-1})(F(u^{\nu+1})) = \left(\hat{A}(u^{\nu+1})\right)^+ \text{ truncation at active nodes}$$

Convergence Results for Non-Smooth Schur Newton Methods

Theorem: (Gräser & Kh. 09, Gräser 09)

global convergence (exact and inexact version) independent of any parameters

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- **locally quadratic convergence** for non-degenerate problems
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- **finite termination**

Interpretations

non-smooth Schur Newton iteration:

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- evaluation of F^{-1} : semilinear elliptic problem (obstacle potential: active set)
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extension and globalization of primal-dual active set strategies: (Gräser 07)

non-smooth Schur-Newton for L^2 -control $\iff$ primal-dual active set (Hintermüller, Ito, Kunisch 03)