Sobolev gradient methods and applications with FreeFem++

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Outline

- The method of Sobolev gradients is used for optimization problems.
- A Sobolev gradient presents an alternative to using the Euler-Lagrange equations.
- The resulting gradient flow often has desirable properties (global existence and asymptotic convergence) in the infinite dimensional setting.
- Very natural formulation in the finite element setting.

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- Suppose ϕ is differentiable, defined on a Hilbert space H
- $u \in H$, there exists a unique $\nabla_H \phi(u) \in H$, so that

$$\phi'(u)h = \langle h, \nabla_H \phi(u) \rangle_H \tag{1}$$

  for all $h \in H$.
- Consider the flow

$$z'(t) = -\nabla_H \phi(z(t)) \text{ and } z(0) = u_0. \tag{2}$$

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- Under certain conditions, one obtains an equilibrium point in the asymptotic limit.
  1. Gradient inequality - there exists $c \in (0, 1)$ and $m > 0$ so that
  $$\|\nabla_H \phi(u)\|_H \geq m\phi(u)^c$$
  for all u in the range of z.
  2. Uniform convexity - there exists a constant $m > 0$ so that
  $$\phi''(u)(h, h) \geq m\|h\|_H^2$$
  for all h.
- If $u = \lim_{t\to\infty} z(t)$ exists, then $\nabla_H \phi(u) = 0$.

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- For $u \in H^1(\Omega)$, let

$$\phi(u) = \int_\Omega \frac{|\nabla u|^2}{2} + f(u)$$

so that

$$\phi'(u)h = \int_\Omega \nabla h \cdot \nabla u + f'(u)h$$

- Find u so that $\phi'(u)h = 0 \; \forall \; h \in H^1$.
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- Find a solution using a minimizing gradient flow.
- Iterate using

$$u_{n+1} = u_n - t_n \nabla E(u_n)$$

- Weak formulation of the L^2 gradient: find v so that

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- What is the relationship between the L^2 and H^1 gradients?
- For $u \in L^2(\Omega)$ and $h \in H^1(\Omega)$,

$$\langle u, h\rangle_{L^2} = \langle (I-\Delta)^{-1} u, h\rangle_{H^1}$$

- and thus

$$\langle h, \nabla_{L^2}\phi(u)\rangle_{L^2} = \langle h, (I-\Delta)^{-1}\nabla_{L^2}\phi(u)\rangle_{H^1}.$$

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- The Gross-Pitaevskii functional for rotating Bose-Einstein condensates

$$\phi(u) = \int_{\mathcal{D}} \frac{|\nabla_A u|^2}{2} + V_{eff}|u|^2 + \frac{g|u|^4}{2}$$

- $$V_{eff}(r) = V_{trap}(r) - \frac{\Omega r^2}{2}$$

- $$\nabla_A u = \nabla u + i\Omega A_L u \text{ with } A_L(x,y) = (y,-x)^t$$

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- Euler-Lagrange equation

$$\phi'(u)h = \int_{\mathcal{D}} h \nabla_{L^2} \phi(u)$$

- $\Rightarrow$ imaginary time evolution.
- Sobolev gradient flow using the standard H^1 inner product and $\langle u, v \rangle_{H_A} = \langle u, v \rangle_{L^2} + \langle \nabla_A u, \nabla_A v \rangle_{L^2}$
- $\Rightarrow$ preconditioned version of imaginary time evolution.

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- Form for the gradient?
- Using the same reasoning as before, we precondition the Euler-Lagrange equations using $(I - \Delta)^{-1}$ and $(I - \nabla_A \cdot \nabla_A)^{-1}$

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- What role does the choice of inner product play on numerical efficiency?
- $f \in L^2(\mathcal{D}, \mathbb{C})$,

$$\phi(u) = \frac{1}{2}\int_{\mathcal{D}} |\nabla u - i\Omega A_L u|^2 + V_{eff}|u|^2 + \frac{g}{2}|u|^4 - (f^* u + f u^*)$$

- Given f, the minimizer u_f can be analytically determined.
- Measure the rate of convergence to the minimizer.

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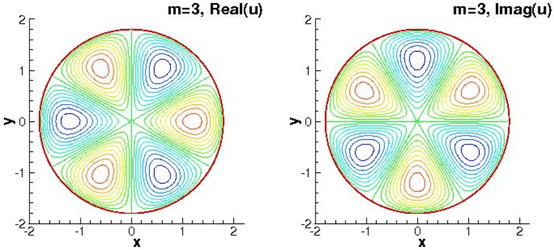

Figure: A contour plot of the minimizer

	M/Triangles	n	CPU	E(u)	δt
L	100/1776	1176	85	-.4934	8e-4
H	100/1776	47	3.4	-.4934	1
H_A	100/1776	14	1	-.4934	3
L	200/7064	4292	1252	-.5025	2e-4
H	200/7064	47	13.8	-.5025	1
H_A	200/7064	14	4.1	-.5025	3
L	400/27604	$>$ 8000	$>$ 9193	-.5027	5e-5
H	400/27604	47	54.2	-.5047	1
H_A	400/27604	14	16.2	-.5047	3

Table: Test case with manufactured solutions. Algorithm efficiency and convergence test for the finite element implementation (fixed time step computation). The triangular mesh is generated with M points on the border of the domain.

- FreeFem++ has an option for mesh adaptivity based on metric control.
- Important for efficiency in problems with rapidly changing structure (i.e. vortex formation).
- Use relative change in energy to trigger mesh adaptivity.
- Compare two mesh adaptivity variables $\xi = |u|$ and $\xi = [u_r, u_i]$.
- Compare using Sobolev gradient method and imaginary time evolution .
- Compare for various initial estimates.

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		SG		IT	
	M	n	CPU	n	CPU
Ad, $\xi = [u_r, u_i]$	200	232	55	139	54
Ad, $\xi = \|u\|$	200	241	44	142	40
No Ad	200	223	72	75	92
No Ad	400	243	315	92	24

Table: Computation for $g = 500, \Omega = 2$ and combined harmonic-plus-quartic trapping potential. Initial condition with six artificially placed vortices. SG is the Sobolev gradient method and IT is imaginary time evolution (Runge-Kutta-Crank-Nicolson).

- Many models in image processing involve solving a minimization problem (i.e. Euler's elastics, TV-Stokes model for inpainting, and Perona-Malik model for diffusion).
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- Currently under investigation: Find a solution to $\nabla^{\perp} u \cdot \nabla \Delta u = 0$ (Navier-Stokes image inpainting)
- by minimizing

$$\phi(u, v) = \int_{\Omega} |\nabla^{\perp} u \cdot \nabla v|^2 + \lambda |\Delta u - v|^2$$

- Compute a gradient in a Sobolev space H^k.
- Compare efficiency with other models.
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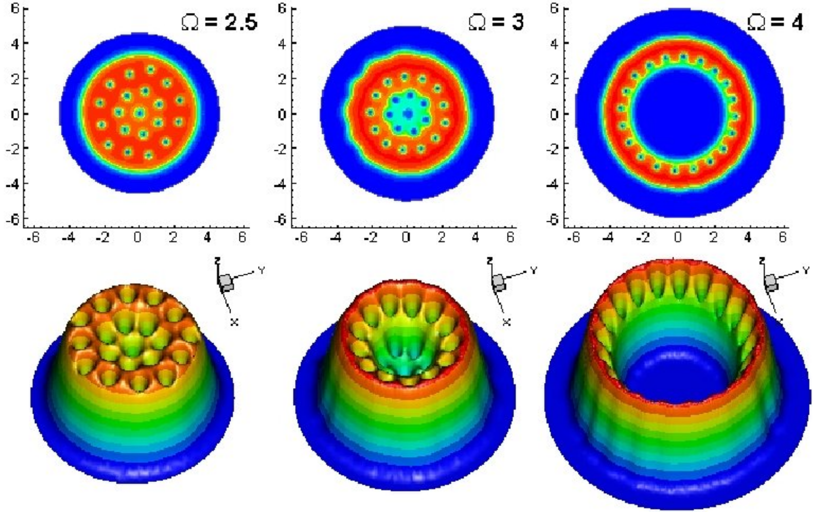

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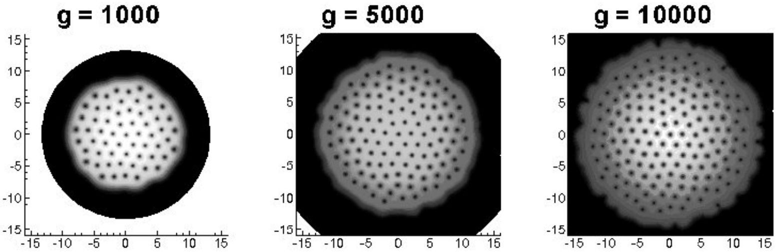
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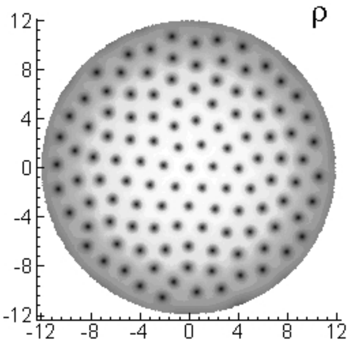
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