Adaptive algorithm for saddle point problem for Phase Field model

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Outline

- Introduction and Motivation
- Shrinking Dimmer Dynamics
- Phase Field model for vesicle shape and shape transition
- Implementation ,adaptivity and example
- On-going works and summary

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Saddle point problem

Predicting the transition/reaction/nucleation rate, as well as the study of the transition state, is of great interest to many areas of applications, such as computational biology, chemical engineering, material science and engineering.

- conformational changes in macromolecules,
- chemical reactions,
- diffusion in condensed-matter systems,
- nucleation phenomena during phase transitions

Difficulties with experimental study: Rare events, unstable and hard to observe.

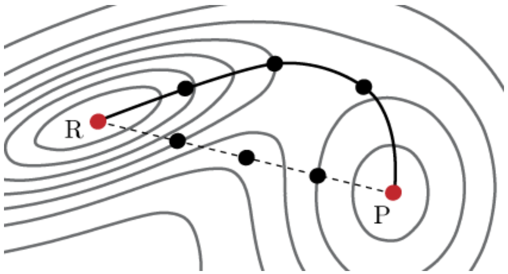
Challenges with Saddle Point Search:

x in Ω, a point/state in the energy landscape;
E(x) an energy functional defined on Ω.

- High dimensionality and complexity of the energy landscape E;
- Unstable nature of the saddle points/transition states;
- Difficult/Expensive to calculate (Hessian).

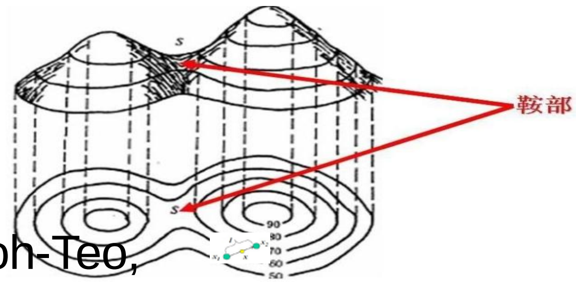
Saddle point algorithms

Chain of States Methods: make use of the information of initial and final states (compute Minimal Energy Paths and transition states)



- Classical minimax method, by Rabinowitz,
- Nudged elastic band, by Henkelman-Jonsson-Uberuaga, etc.
- String method, by E-Ren-Vanden Eijnden, etc.

Surface Walking Algorithms: use only local quantities around one point on the potential energy surface (compute transition states)



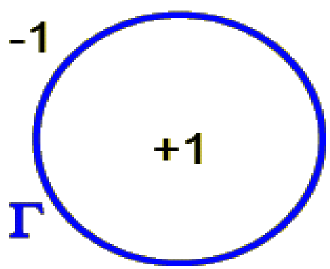
- Eigen-following method, by Cerjan-Miller,
- Step and slide method, by Miron-Fichthorn,
- Trajectory following algorithms, by Grantham and Vincent-Goh-Teo,
- Activation-relaxation technique method, by Mousseau-Barkema,
- Gentlest ascent method/dynamics, by Crippen-Scheraga, E-Zhou, E-Samanta,
- Dimer method/dynamics, by Henkelman-Jonsson, Poddey-Blochl, etc.

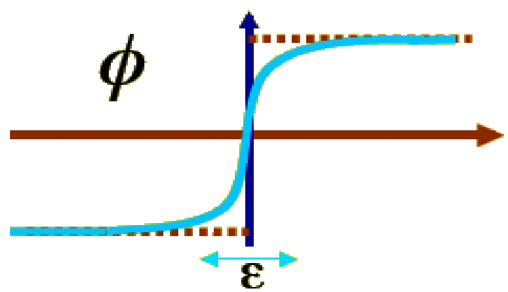
Phase Field Model

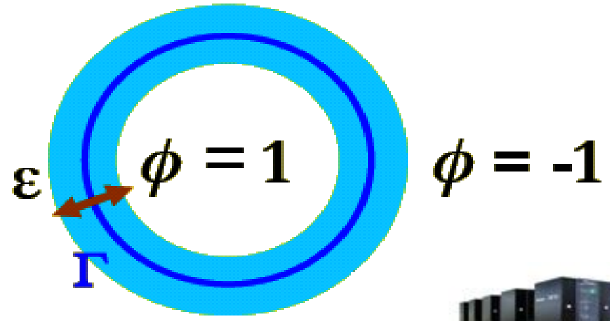
Diffuse interface description of surfaces/interfaces, idea goes back more than 100 years (van de Waals, Chem. Phys. 1894)

Ginzburg-Landau, Cahn-Hilliard, Halperin-Hohenberg,…

- A popular approach for free/moving interface problems
  physics, biology, chemistry etc.
- Sharp interfaces → diffuse interfaces characterized by some order parameters (phase field functions)





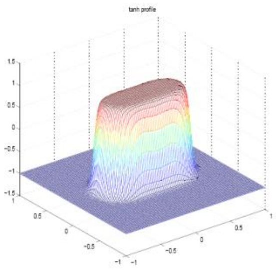


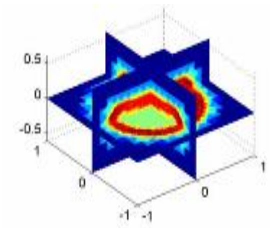
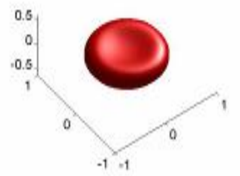
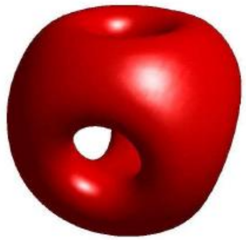
Phase Field Model

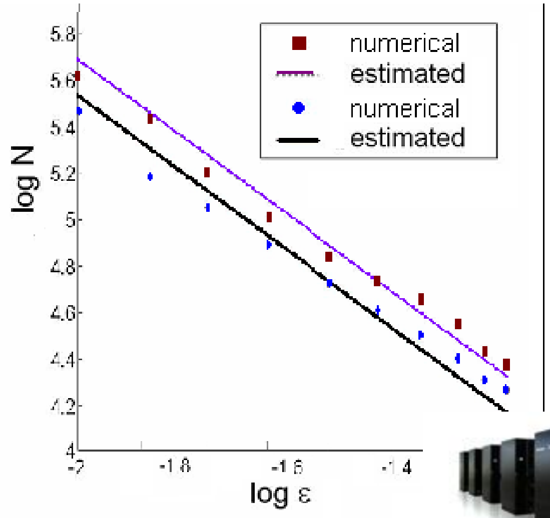
- Handle complex topological changes naturally.
  solve a single set of equations with smooth solutions.

- Computationally challenging:
  2D surface → 3D phase function
  Thin interface layer → high spatial resolution and stiffness

- Adaptivity can help reducing the computational cost.



Eg: Du -Zhang, SISC, 2008
3D computation with effectively 2D complexity

Motivation

- Shape (interfaces) often go through topological changes during transition.

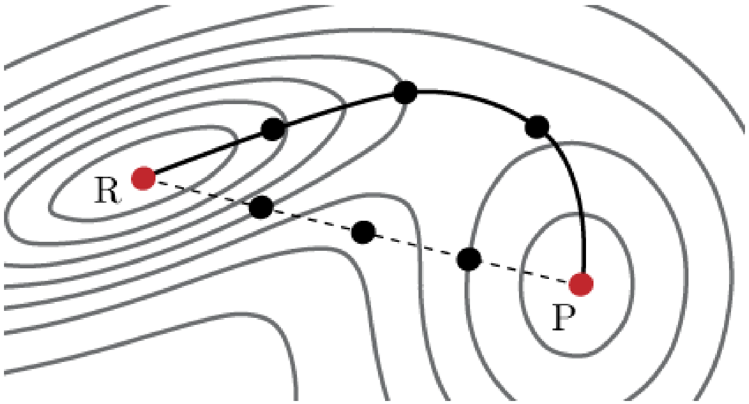
    Phase Field Model handles topological change well

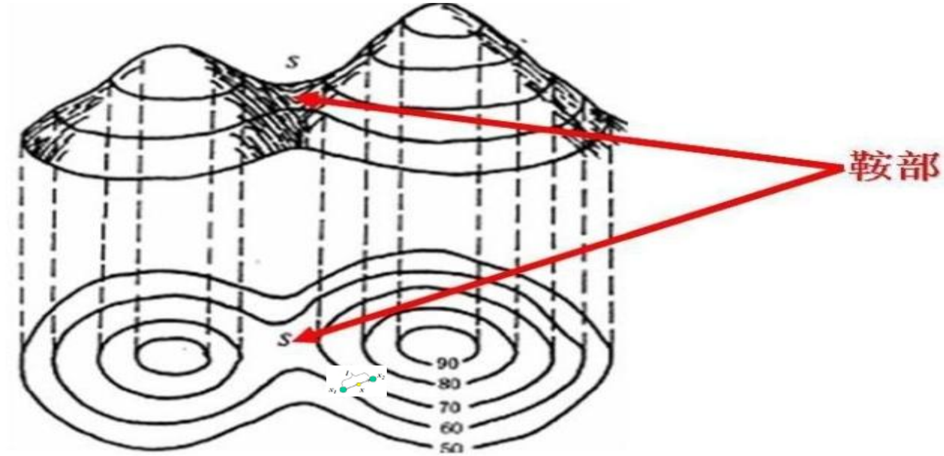
- Quantitative study of transition/reaction/nucleation rate require high accuracy.

    Thus, very thin interface and high spatial resolution.

- Adaptivity reduces in orders of magnitude the computational cost.

Chain of states or surface walking?





- Evolve many states (phase functions) simultaneously.
- Frequent inter-state communication and interpolation.
- hard to adapt mesh to solutions and parallelize efficiently.

- Evolve single state and related unstable direction.
  highly efficient adaptive mesh.
- Can be parallelized using domain decomposition.
  same as solving other PDE's.

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GAD and dimmer method

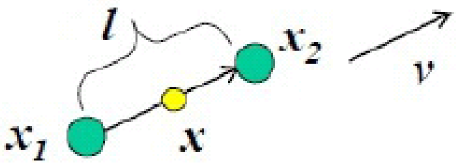
Gentlest ascent method/dynamics, by Crippen-Scheraga, E-Zhou, E-Samanta,

Finding index-1 saddle point of V(x).

$$\dot{x} = -\nabla V(x) + 2(\nabla V, v)v \qquad \dot{v} = -\nabla^2 V(x)v + \frac{(v, \nabla^2 V v)}{(v, v)} v$$

Dimmer method/dynamics, by Henkelman-Jonsson, Poddey-Blochl, etc.

$$\dot{x} = (I - 2vv^T)F_\alpha \qquad \dot{v} = (I - vv^T)(F_1 - F_2)/l$$



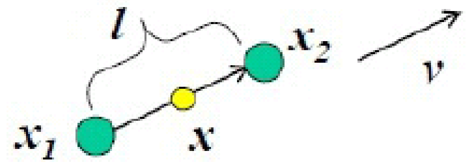
where $F_\alpha=(2-\alpha)F_1+(\alpha-1)F_2$, and $F_i= -\nabla V(x_i)$ for i=1,2.

Shrinking Dimmer Dynamics

$$\dot{x} = (I - 2vv^T)F_\alpha$$

$$\dot{v} = (I - vv^T)(F_1 - F_2)/l$$

$$\dot{l} = -\Gamma'(l)$$



with $x(0)=x_0$, $v(0)=v_0$, $l(0)=l_0$ and $||v_0||_2 = 1$, $l_0 > 0$.

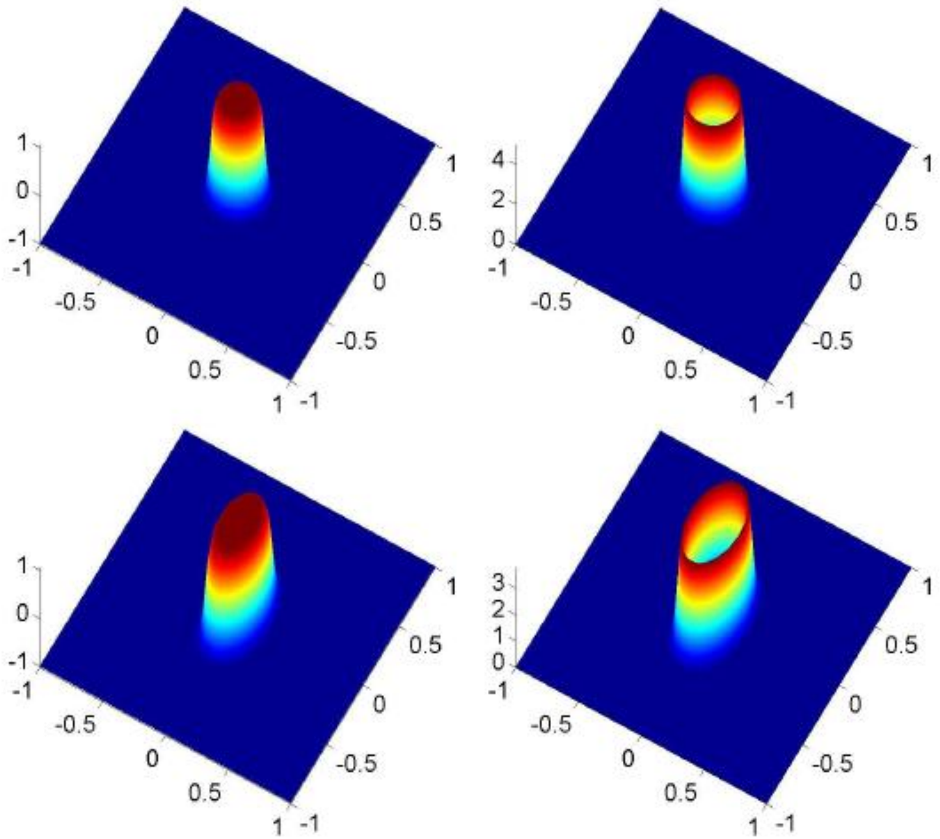
Theorem. (x^*, v^*, l^*) is a linearly stable steady state of the above SDD, if and only if

- x^* is a index-1 saddle point of the energy V.
- v^* is a unit eigenvector of the Hessian of V at x^*, $H_V(x^*)$, that correspond to the smallest and only negative eigenvalue.
- l* is 0.

(Zhang-Du,SISC,2012)

SDD applied to Phase Field

Infinite dimensional problem: the computation of critical nuclei (left) and unstable direction (right) with isotropic (upper) / anisotropic (lower) interfacial energy.



Reproduced the results in
(Zhang-Chen-Du, PRL, 2007), calculated using NEB method.

SDD with constraints

The challenging task of searching for saddle points may be further complicated by additional constraints imposed on configuration variables (e.g., fixed bond length, conserved order parameter, ...).

Let the constraints be denoted by G(x) = 0.

Idea: Enforce constraints on x and move v along the tangential space of G.

Let $J = \nabla G^T$ whose columns are the normal vectors of the level surfaces correspond to the constraints. The tangential projection operator

$$P(G) = I - J[J^T J]^{-1} J^T$$

project force onto the tangential space of G

$$\tilde{F}_\alpha = P(G_\alpha) F_\alpha$$

SDD with constraints

Constrained SDD:

$$\dot{x} = (I - 2vv^T)\tilde{F}_\alpha$$

$$\dot{v} = (I - vv^T)(\tilde{F}_1 - \tilde{F}_2)/l + J\beta$$

$$\dot{l} = -\Gamma'(l)$$

(Zhang-Du,JCP,2012)

The initial conditions satisfy the following compatibility assumptions

$G(x_0)=0$, $||v_0||=1$ and $J_0 v_0=0$.

Here the dynamically updated Lagrange multiplier β has the following form in general

$$\beta = -[J^T J]^{-1} v^T H_G(x)\dot{x}$$

Remarks

- β=0 for linear constrains
- β= $-[J^T J]^{-1}(J_1 - J_2)^T \dot{x}$ for quadratic constrains

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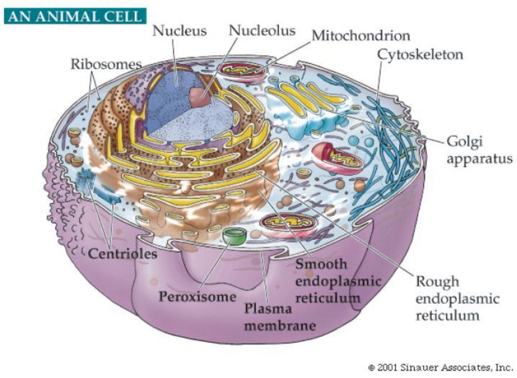
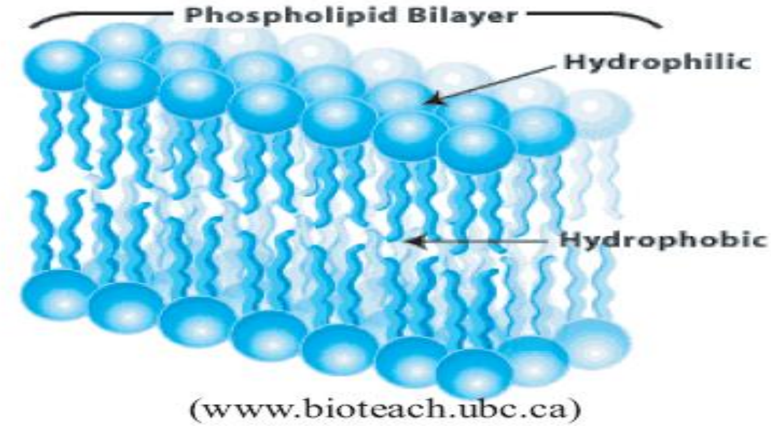
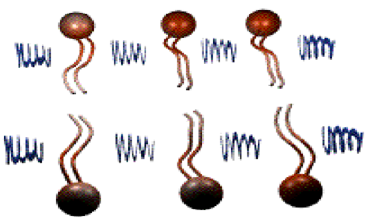
Vesicle membrane model





Elastic bending energy, (Helfrich 1973)

$$E_{el} = \int_{\Gamma} H^2 ds$$

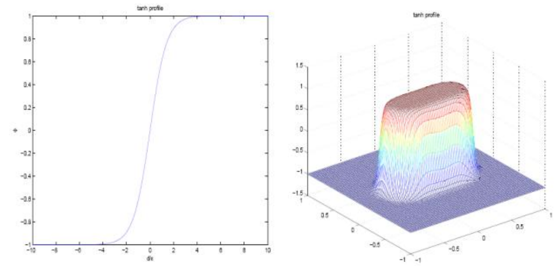


With volume and surface area constraints.

Phase field formulation

Energy functional

$$E(\phi) = \frac{3\sqrt{2}}{8}\int_{\Omega}\frac{\kappa\varepsilon}{2}(\Delta\phi - \frac{1}{\varepsilon^2}(\phi^2 - 1)\phi)^2 d\Omega$$



as $\varepsilon \to 0$,

$$\phi \to \tanh(\frac{d}{\sqrt{2}\varepsilon}) \quad \text{and} \quad E(\phi) \to E_{el}$$

Where d is the signed distance function of the membrane.

$$V(\phi) = \int_{\Omega}\phi d\Omega \to v_{in} - v_{out} \quad \text{and} \quad S(\phi) = \int_{\Omega}(\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{4\varepsilon}(\phi^2 - 1)^2)d\Omega \to \frac{2\sqrt{2}|\Gamma|}{3}$$

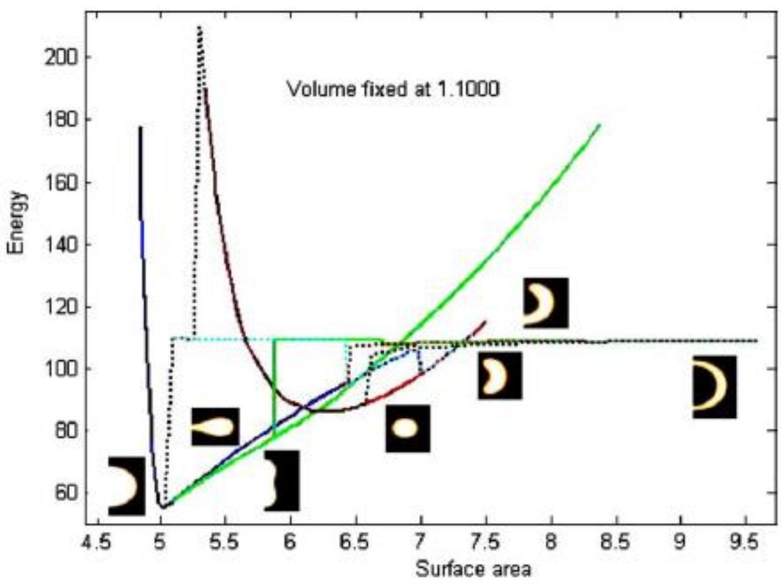
(Du-Liu-Wang,JCP,2004)

Equilibrium (stable, meta-stable state) of the vesicle.

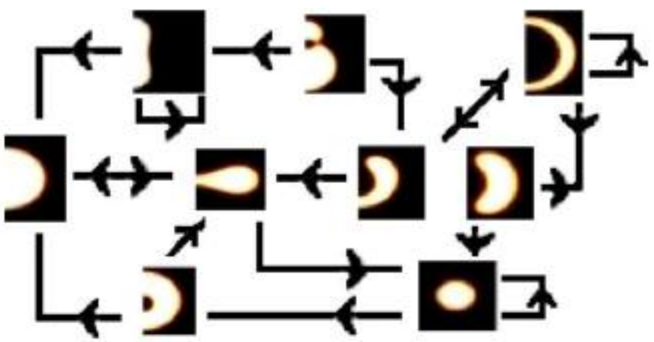
- Minimize E with constraints on V and S.(axial symmetry)(2004)
- 3D simulation with adaptive FEM(Du-Zhang,SISC,2008)(Zhang-Das-Du,JCP,2009)

Shape transition

Many solution branches, i.e. many stable or meta stable states with the same volume and surface area. Eg. Axial symmetric case (Du-Liu-Wang,JCP,2004)



Solution paths



The energy landscape is even more complicated in non-axial-symmetric case. We are interested in

- The configuration of the transition states (saddle points of E(φ)).
- The energy barrier of the shape transition.

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Algorithm

Constrained SDD

$$\mu_1 \dot{\phi} = (I - 2vv^T)\tilde{F}_\alpha$$

$$\mu_2 \dot{v} = (I - vv^T)(\tilde{F}_1 - \tilde{F}_2)/l + J\beta$$

$$\mu_3 \dot{l} = -\Gamma'(l)$$

$$G(\phi) = \begin{pmatrix} V(\phi) - A \\ S(\phi) - B \end{pmatrix} = 0$$

Here the notation vv^T usually used in linear algebra is interpreted as $vv^Ty=v^Tyv$, for any v in H and y in H^* with $v^Ty=y^Tv$ denote the dual pairing of v with y.

A and B are given according to the volume and surface area constraints, and Γ is taken to be $\frac{l^4}{4}$.

Algorithm

The gradient of E is interpreted as the first variation of E(φ) with respect to φ

$$\nabla E = \frac{\delta E(\phi)}{\delta \phi} = \kappa \varepsilon \Delta f - \frac{\kappa}{\varepsilon}(3\phi^2 - 1) f$$

where

$$f = \Delta \phi - \frac{1}{\varepsilon^2}(\phi^2 - 1)\phi$$

Similarly

$$J = \nabla G^T = (1 \quad -\varepsilon f) \qquad J^T J = \begin{pmatrix} |\Omega| & -\varepsilon \int f \\ -\varepsilon \int f & \varepsilon^2 \int f^2 \end{pmatrix}$$

In order to avoid calculating Hessian of spatial derivatives of φ, the constraint on surface area is splitted into two parts when updating β.

$$S(\phi) = S_1 + S_2 = \frac{\varepsilon}{2}\int |\nabla \phi|^2 + \frac{1}{4\varepsilon}\int (\phi^2 - 1)^2$$

Recall $\beta = -\mu_1^{-1}\mu_2 [J^T J]^{-1} v^T H_G(x)\dot{x}$, the second component of $v^T H_G \dot{x}$ is

calculated as $\int (\nabla S_1(\phi_1) - \nabla S_1(\phi_2))\,\dot{x} + \int \frac{1}{\varepsilon} v(3\phi^2 - 1)\dot{x}$

Discretization

■Temporal: Forward Euler

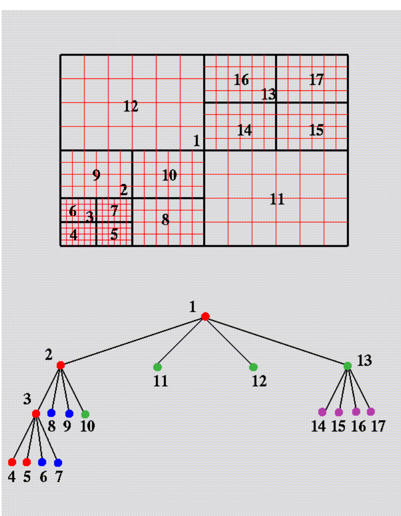
➢with renormalization of v after updating

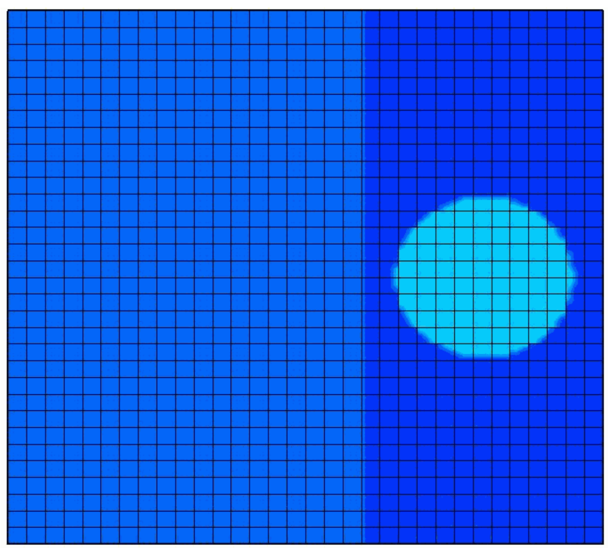
➢also implemented an alternative constraint enforcement scheme based on time splitting, projection and normalization.

■Spatial: Finite difference on oct-tree block structured adaptive mesh

➢Builds on PARAMESH (parallel AMR software package)

➢refine-coarsen criterion designed base on interface capturing and gradient test.



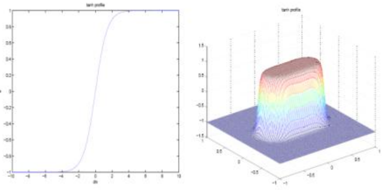


PARAMESH
MacNeice,Olson,Mobarry et al.
Comp. Phys. Comm.,2000

Refine-coarsen criterion

Recall

$$\phi \approx \tanh\left(\frac{d}{\sqrt{2}\varepsilon}\right)$$



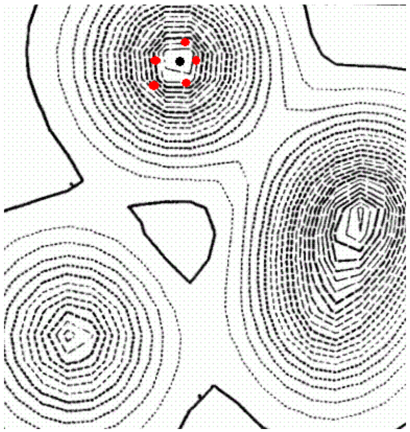
The distance of a point to the interface can be easily estimated using the value of φ. We simply set thresholds on the distance to determine whether the grid should be refined or coarsened according to φ.

for v:

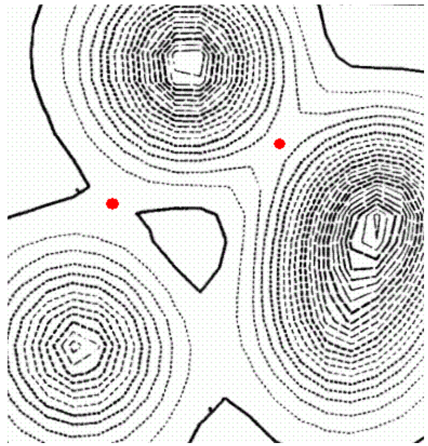
- In addition to φ , we set a threshold on $|\nabla v|$ to determine if the gird should be refined.
- Notice v= $(\varphi_2 - \varphi_1)/l$, and the difference between φ_1, φ_2 and φ are mainly in the interface region when the SDD is about to converge. The variation of v also concentrates near the interface, as we observed both in (Zhang-Du,SISC,2012) and current simulations.
- The threshold is applied when l is sufficiently small.

Saddle searching strategy

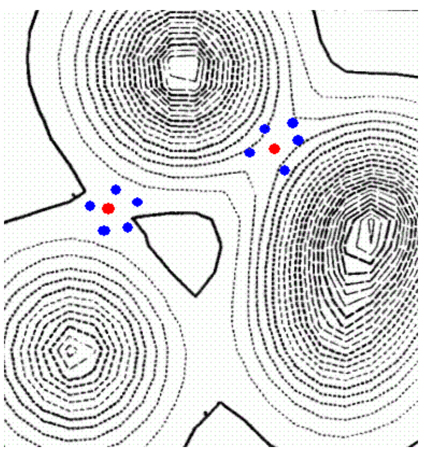
- red walkers follow SDD
- blue walkers follow gradient flow
- walkers can be parallelized naturally



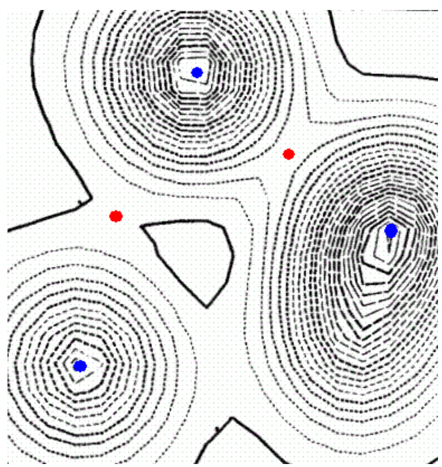
initialize red walkers



find saddles

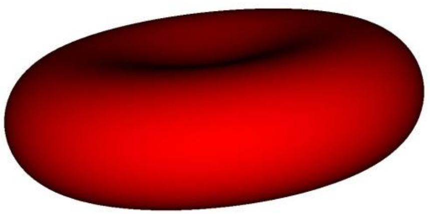


initialize blue walkers

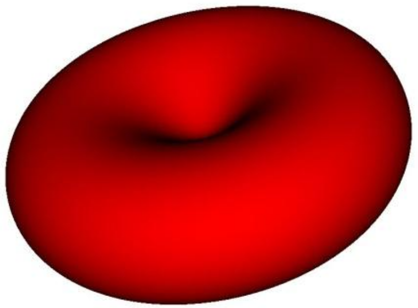


find minima

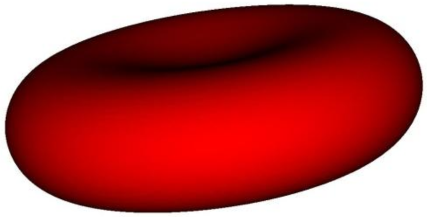
Numerical example



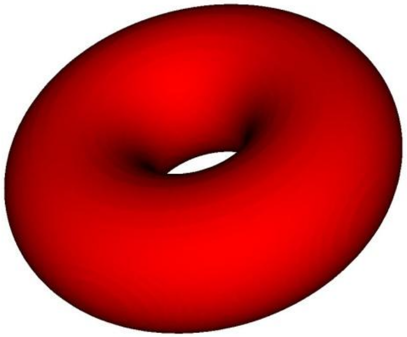
Initial state



transition state

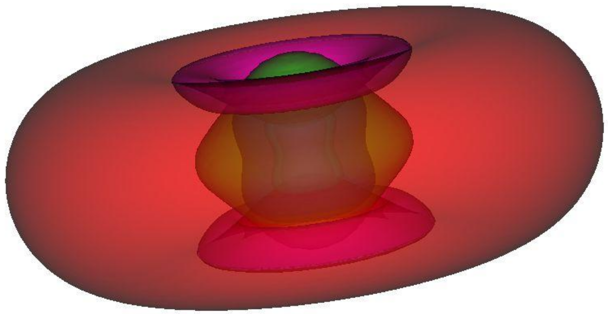


(meta)stable state

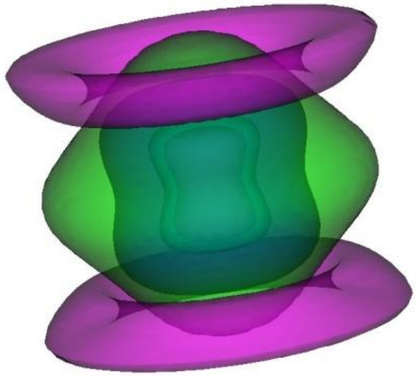


stable state

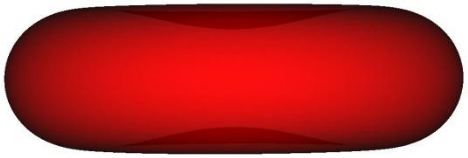
Numerical example



Transition state and unstable direction

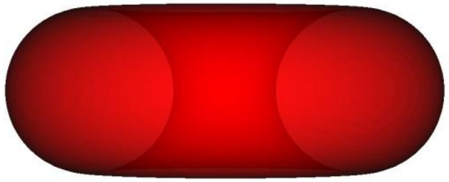


unstable direction



Eng=17.22

Eng=18.33



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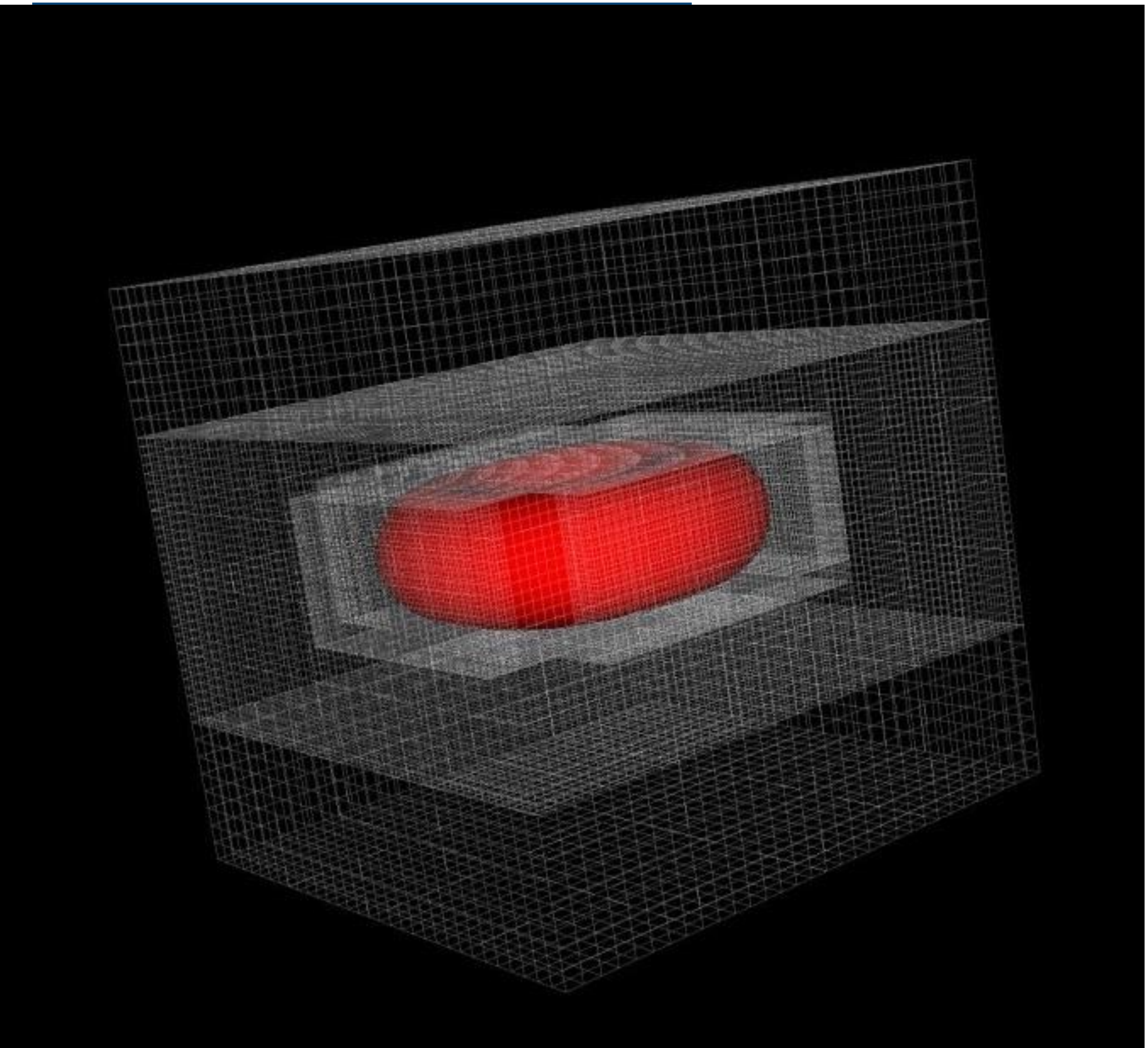
Numerical example



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On-going and future works

On-going works

- Algorithms
  - multi-stage/multi-step methods, adaptive time steps.
  - high-order index saddle point
- Applications
  - material science, nucleation
  - vesicle membrane, high genus transition state

Future works

- (semi)-implicit time stepping based on multi-grid solver on adaptive mesh.
- adaptive dimmer length
- rigorous analysis of adaptivity both in time and space under finite element framework
- Large scale adaptive SDD simulation

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special research funds for State Key Lab., Y22612A33S,2012-2013

Summary

- Saddle point search is interesting and challenging.
  - high dimensionality
  - instability

- Shrinking Dimmer Dynamics (SDD):
  - converts instability to a stable system
  - guarantees convergence
  - requires only first-order derivatives
  - suitable for parallel adaptive mesh
  - walkers are independent

- Much more work is on the way.

Thank You!