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Mittuniversitetet

MID SWEDEN UNIVERSITY

# DFPM
# The Dynamic Functional Particle Method

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# DFPM SOLVES EQUATIONS

We solve the abstract equation

$$\mathcal{F}(v) = 0$$

by solving the oscillating damped equation

$$\mu u_{tt} + \nu u_t = \mathcal{F}(u)$$

with mass parameter $\mu$ and damping parameter $\nu$

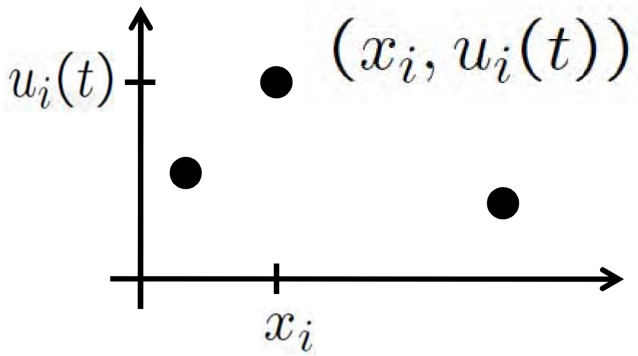
such that

$$u_t, u_{tt} \to 0$$

# DISCRETIZE IN SPACE

Discretize using finite differences, finite elements, or…

then $u_i(t) \approx u(x_i, t)$




giving the finite dimensional dynamical system

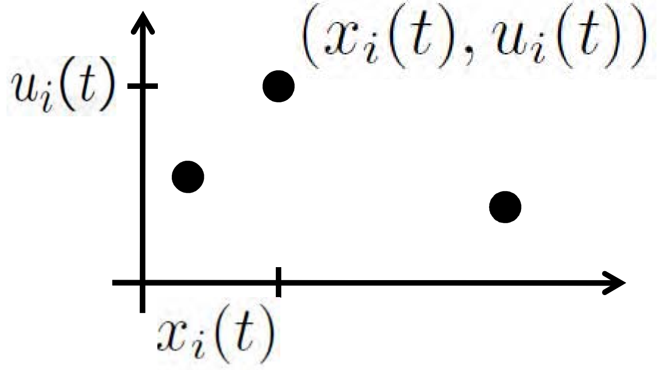
$$\mu_i \ddot{u}_i + \nu_i \dot{u}_i = F_i(x_1, \ldots, x_n, u_1 \ldots, u_n)$$

with mass and damping parameters

$$\mu_i = \mu(x_i, u_i(t), t),\ \nu_i = \nu(x_i, u_i(t), t)$$

# MESH FREE METHOD

Particles may be chosen free to move




Giving the DFPM

$$\mu_i \ddot{u}_i + \nu_i \dot{u}_i = F_i(x_1(t), \ldots, x_n(t), u_1(t) \ldots, u_n(t))$$

For example (no grid assumed)

$$\frac{d^2u}{dx^2}(x_i) \approx \left( \frac{\triangle x_{i+1}}{\langle x_i \rangle} u_{i-1} - 2u_i + \frac{\triangle x_i}{\langle x_i \rangle} u_{i+1} \right) / \triangle x_{i+1} \triangle x_i$$

$$\triangle x_i = x_i - x_{i-1}, \langle x_i \rangle = \frac{x_i + x_{i+1}}{2}$$

# A FIRST EXAMPLE

As an introductory example consider the nonlinear initial value ODE

$$\frac{dv}{dx} = xv^2, v(0) = 0$$

That will give the nonlinear PDE (note the sign)

$$\mu u_{tt} + \nu u_t = -u_x + xu^2$$

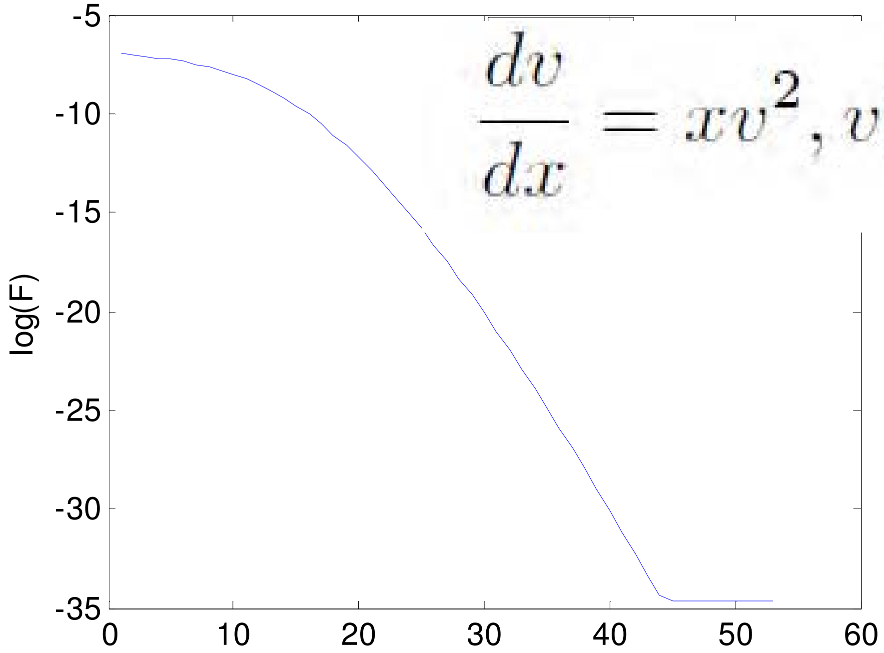
Using backward finite differences on a fixed grid gives DFPM

$$\mu_i \ddot{u}_i + \nu_i \dot{u}_i = -\frac{(u_i - u_{i-1})}{h} + x_i u_i^2$$

# A FIRST EXAMPLE DYNAMICS...

Solution in $x \in [0, 1]$

with parameters $\mu = 1, \nu = 20$




$$\frac{dv}{dx} = xv^2, v(0) = 0$$

The **convergence is exponential**

# FIRST ORDER SYSTEM

Solve the ODE for the particle system

$$\mu_i \ddot{u}_i + \nu_i \dot{u}_i = F_i(x_1, \ldots, x_n, u_1 \ldots, u_n)$$

by solving the first order system

$$\dot{u}_i = w_i$$

$$\dot{w}_i = -\frac{\nu_i}{\mu_i} w_i + \frac{1}{\mu_i} F_i(x_1, \ldots, x_n, u_1 \ldots, u_n)$$

# USE SYMPLECTIC SOLVER FOR THE SYSTEM

Symplectic Euler (one of two) is

$$w_i^{k+1} = w_i^k - \triangle t_k \frac{\nu_i}{\mu_i} w_i + \triangle t_k \frac{1}{\mu_i} F_i(x_1, \ldots, x_n, u_1^k \ldots, u_n^k)$$

$$u_i^{k+1} = u_i^k + \triangle t_k w_i^{k+1}$$

- **Conserves energy** if no damping is added
- Very **fast and stable**
- **Extrapolation** can be performed easily

# A NONLINEAR BOUNDARY VALUE ODE

The equation

$$\frac{d^2v}{dx^2} + v\frac{dv}{dx} = \sin(x)(\cos(x) - \frac{2}{\pi} - 1) - \frac{2}{\pi}x\cos(x)$$

$$v(0) = v(1) = 0$$

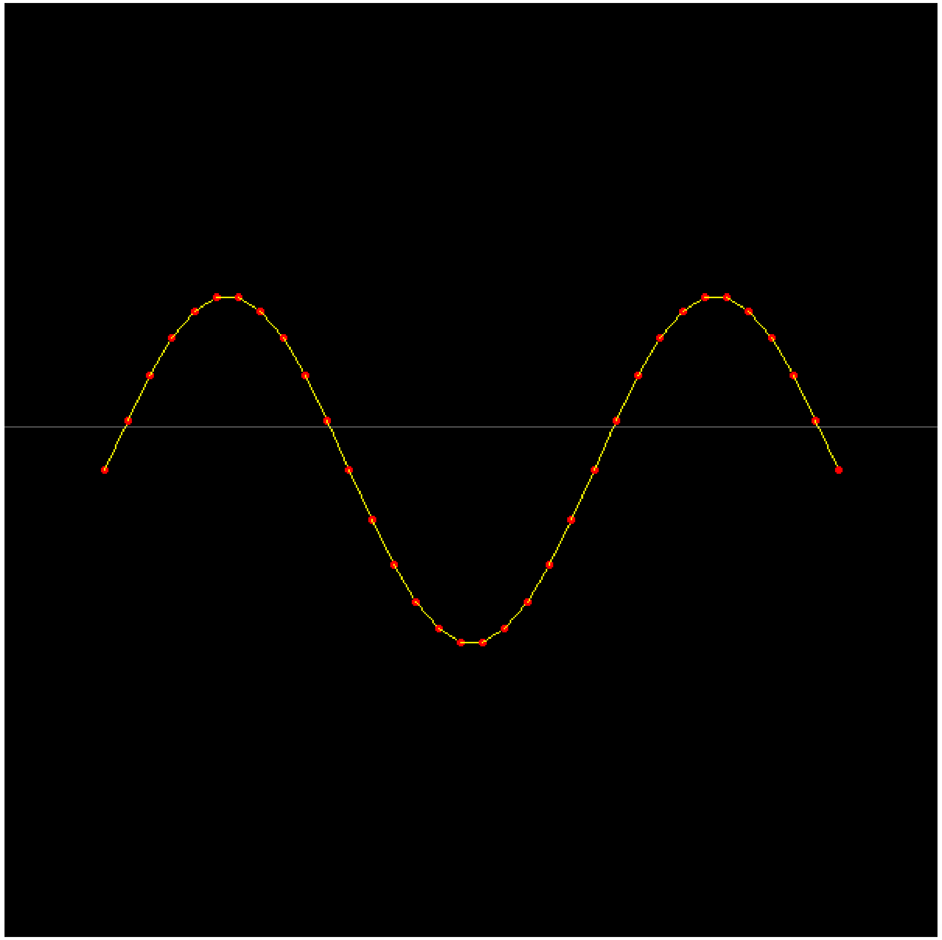
The infinite dimensional dynamical system

$$\mu u_{tt} + \nu u_t = u_{xx} + uu_x + g(x)$$

DFPM

$$\mu_i \ddot{u}_i + \nu_i \dot{u}_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + u_i \frac{u_{i+1} - u_{i-1}}{2h} + g(x_i)$$

Animation of $\mu_i \ddot{u}_i + \nu_i \dot{u}_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + u_i \frac{u_{i+1} - u_{i-1}}{2h} + g(x_i)$



# ENERGY AND POTENTIAL

If the 'force field' is **conservative** there exists a potential

$$V = -\sum_i \int_{u_i} F_i du_i + \sum_{i \neq j} \int_{u_j} F_i du_j + \ldots$$

such that the **minimum of the potential** is the solution of the discretized equations

$$\frac{\partial V}{\partial u_i} = -F_i = 0 \qquad \text{or} \qquad \nabla_{\mathbf{u}} V = -\mathbf{F}(\mathbf{u}) = 0$$

This **global property** can be used in DFPM in a similar way as for simulated annealing…

# ALGORITHMIC IDEAS

Consider the energy functional or Lyapunov function

$$E = T + V = \frac{1}{2}\sum \mu_i \dot{u}_i^2 + V(u_1, u_2, \ldots)$$

then

$$\frac{dE}{dt} = -\sum_i \nu_i \dot{u}_i^2 \leq 0$$

and the damping will always lower the energy functional until it reaches a steady state where the potential is at a minimum.

# ALGORITHMIC IDEAS

**Start** in the direction of lower potential

$$\mathbf{w}^0 = \gamma \mathbf{F}$$

Do **undamped** oscillations to catch a low potential

If **close to a low potential then damp** the system heavily to reach a (local) minimum

Otherwise **systematically lower the energy functional** to reach steady state

# SCHRÖDINGER EQUATION
# THE EIGENVALUE PROBLEM

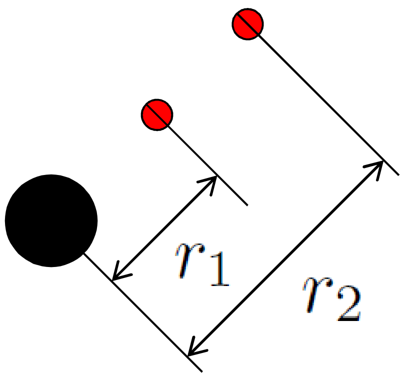
The equation for Helium ground state reads

$$-\frac{\hbar^2}{2m}\Delta\psi + V(r_1, r_2)\psi = E\psi$$

By discretizing in $r_1$ and $r_2$ we get

$$A\mathbf{v} = \lambda\mathbf{v}$$

where $$\|\mathbf{v}\| = 1$$



# SCHRÖDINGER EQUATION
# THE EIGENVALUE PROBLEM

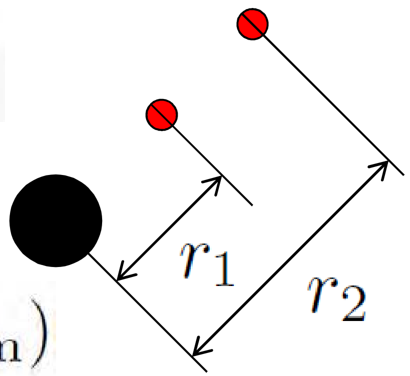
The eigenvalue is not known but can be approximated with the Rayleigh quotient $\mathbf{u}^T A\mathbf{u}$

and DFPM is

$$A\mathbf{u} - \left(\mathbf{u}^T A\mathbf{u}\right)\mathbf{u} = M\ddot{\mathbf{u}} + N\dot{\mathbf{u}}$$

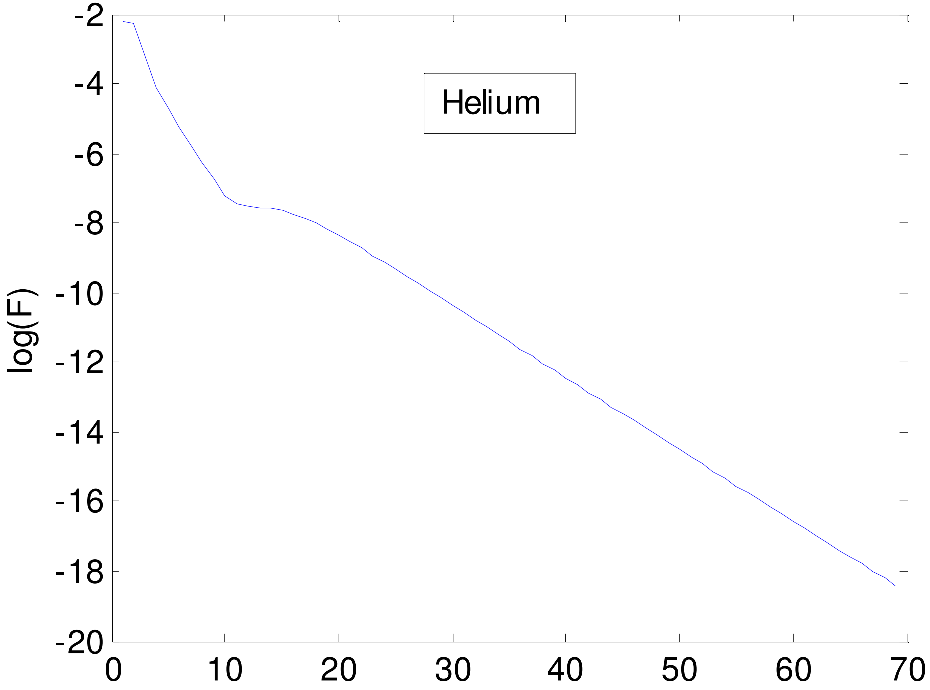
where $||\mathbf{u}|| = 1$ and

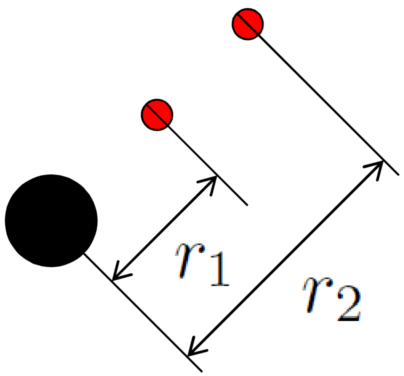
$$M = \mathrm{diag}(\mu_1, \ldots, \mu_{\mathrm{m}}),\ N = \mathrm{diag}(\nu_1, \ldots, \nu_{\mathrm{m}})$$




Deflation is needed for the other eigenvalues

# SCHRÖDINGER EQUATION
# THE EIGENVALUE PROBLEM




The **convergence is exponential**

# NONLINEAR SCHRÖDINGER EQUATION

A nonlinear ODE on the form

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + \hbar^2 \left|x\right|^2 \psi + \omega\psi - \lambda\psi \left|\psi\right|^2 = 0$$

where

$$\omega = \int_{\infty}^{\infty} \psi\left(-\frac{1}{2}\frac{d^2\psi}{dx^2} + \hbar^2 \left|x\right|^2 \psi + \omega\psi - \lambda\psi \left|\psi\right|^2\right) dx$$

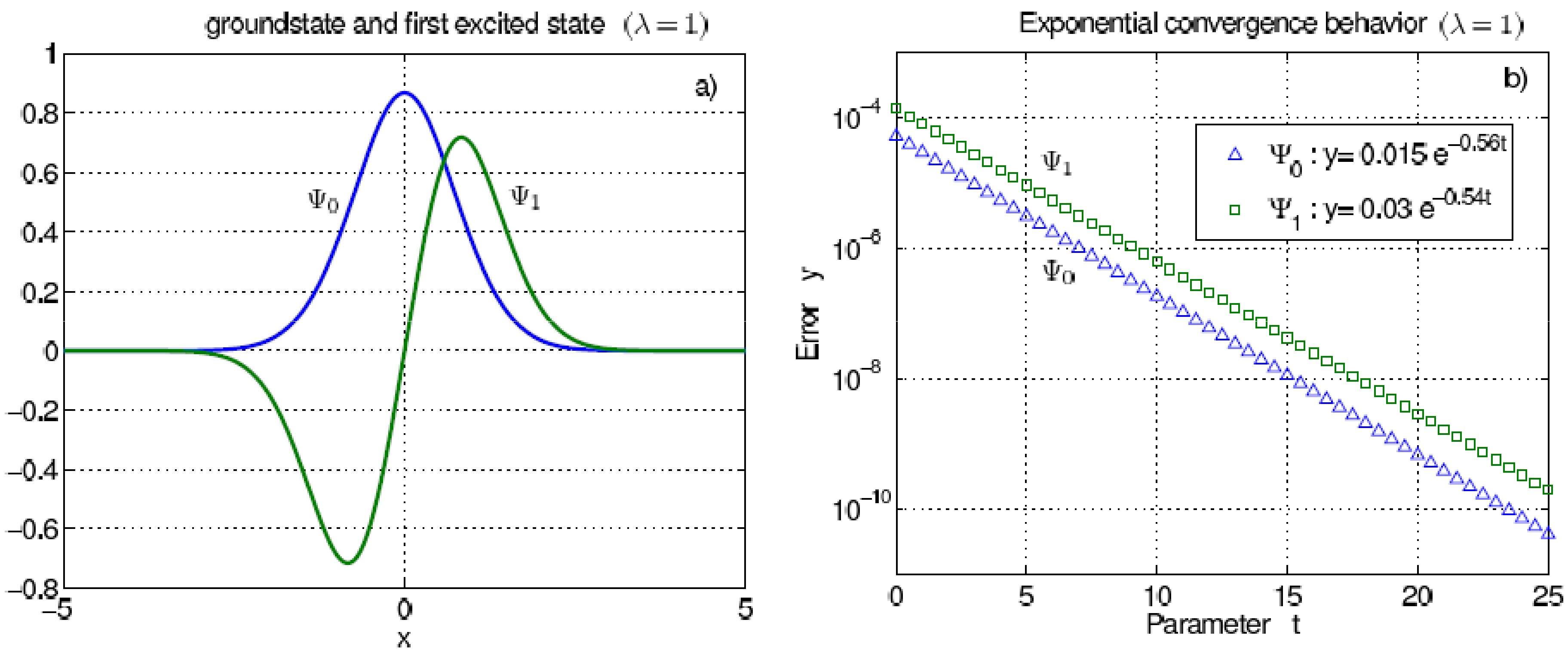
# NONLINEAR SCHRÖDINGER EQUATION

After discretization with finite differences we get the DFPM

$$M\ddot{\mathbf{u}} + N\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u})$$

where $u_i \rightarrow \psi(x_i)$ and $\mathbf{f}(\mathbf{u})$ is a nonlinear function

# NONLINEAR SCHRÖDINGER EQUATION



# CONVERGENCE ANALYSIS

**If** there exist a **potential** every extreme point is a solution of the equations

$$F_i = 0$$

Thus **DFPM always converges** close to a local minium (or maximum with a change of sign)

However, the existence is sufficient but **not a necessary condition** for convergence (e.g., IVP)

**We have not yet failed in solving an equation with the DFPM** (a reformulation of the problem may be necessary)

# CONLUCLUSIONS

•Simple way of solving nonlinear ode, pde,…

•Exponential convergence

•Global convergence properties

# A LOT OF FUTURE WORK

- Extend to several dimensions generally
- Develop time dependent ’mesh’
- Solve the many particle Schrödinger equation (Litium)
- A general method utilizing potential and global properties
- Show mathematically strict the convergence (rate)