4th SPHERIC Workshop
Ecole Centrale Nantes
26 May 2009

The accuracy of SPH approximations

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What is accuracy and why do we care?

We want **convergence** :

$$\lim_{\substack{N\to\infty \\ \Delta t\to 0}} \begin{pmatrix} \text{numerical} \\ \text{solution} \end{pmatrix} = \begin{pmatrix} \text{exact solution} \\ \text{to PDE} \end{pmatrix}$$

The Lax Equivalence Theorem (crude version):

consistency + stability ⇒ convergence

Hirsch (1990), Leveque (2002)

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What is accuracy and why do we care?

The Lax-Wendroff Theorem:

convergence + **conservation** $\Rightarrow$ **weak solution to PDEs**

Without conservation, we might convervge, but maybe not to a real solution.

- shocks
- astrophysics (Monaghan, 2005)

Conservation

Momentum equation:

$$\frac{D\mathbf{u}_a}{Dt} = \sum_b \left(\frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ab} m_b$$

notation:

$$\nabla W_{ab} = \nabla W(\mathbf{x} - \mathbf{x}_a, h)\Big|_{\mathbf{x}=\mathbf{x}_b}$$

Force on *a* due to *b*: $\left(\frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ab} m_a m_b$

Force on *b* due to *a*: $\left(\frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ba} m_a m_b = -\left(\frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ab} m_a m_b$

Equal and opposite if:

- ***W* is symmetric**
- ***h* is uniform**

Not so clear for mass.

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Equivalence of the SPH mass conservation forms

Vaughan *et al*. (2008)

The summation form:

$$\rho_a = \sum_b W\left(\mathbf{x}_b - \mathbf{x}_a\right) m_b$$

Differentiate wrt *t*:

$$\frac{d\rho_a}{dt} = \sum_b \frac{d}{dt} W\left(\mathbf{x}_b(t) - \mathbf{x}_a(t)\right) m_b$$

$$= \sum_b \left[\frac{d\mathbf{x}_b}{dt} \bullet \nabla_b W\left(\mathbf{x}_b - \mathbf{x}_a\right) + \frac{d\mathbf{x}_a}{dt} \bullet \nabla_a W\left(\mathbf{x}_b - \mathbf{x}_a\right) \right] m_b$$

$$= \sum_b \left[\frac{d\mathbf{x}_b}{dt} \bullet \nabla_b W\left(\mathbf{x}_b - \mathbf{x}_a\right) - \frac{d\mathbf{x}_a}{dt} \bullet \nabla_b W\left(\mathbf{x}_b - \mathbf{x}_a\right) \right] m_b$$

$$\frac{d\rho_a}{dt} = \sum_b \left(\frac{d\mathbf{x}_b}{dt} - \frac{d\mathbf{x}_a}{dt} \right) \bullet \nabla_b W\left(\mathbf{x}_b - \mathbf{x}_a\right) m_b$$

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Equivalence of the SPH mass conservation forms

rate of change of summation form density:

Vaughan *et al.* (2008)

$$\left(\frac{d\rho_a}{dt}\right)^{n} = \sum_b \left(\mathbf{u}_b^n - \mathbf{u}_a^n\right) \bullet \nabla_b W\left(\mathbf{x}_b^n - \mathbf{x}_a^n\right) m_b$$

"continuity" form:

$$\left(\frac{d\rho_a}{dt}\right)^{n+\frac{1}{2}} = \sum_b \left(\mathbf{u}_b^n - \mathbf{u}_a^n\right) \bullet \nabla_b W\left(\mathbf{x}_b^n - \mathbf{x}_a^n\right) m_b$$

The two forms would be identical if we had exact time integration!

Conservation and non-uniform *h*

Errors due to $h = h(x,t)$ studied by Hernquist (1993) – important in astrophsyics – errors $\sim 10\%$

$$h = h(x,t) \qquad \Rightarrow \qquad \nabla W(\mathbf{x},h) = \nabla W(\mathbf{x},h)\big|_h + \frac{\partial W(\mathbf{x},h)}{\partial h}\nabla h$$

Additional terms can be derived – 10% CPU time cost.

Nelson and Papaloizou (1994)

"It seems one cannot have everything."

Monaghan (1992)

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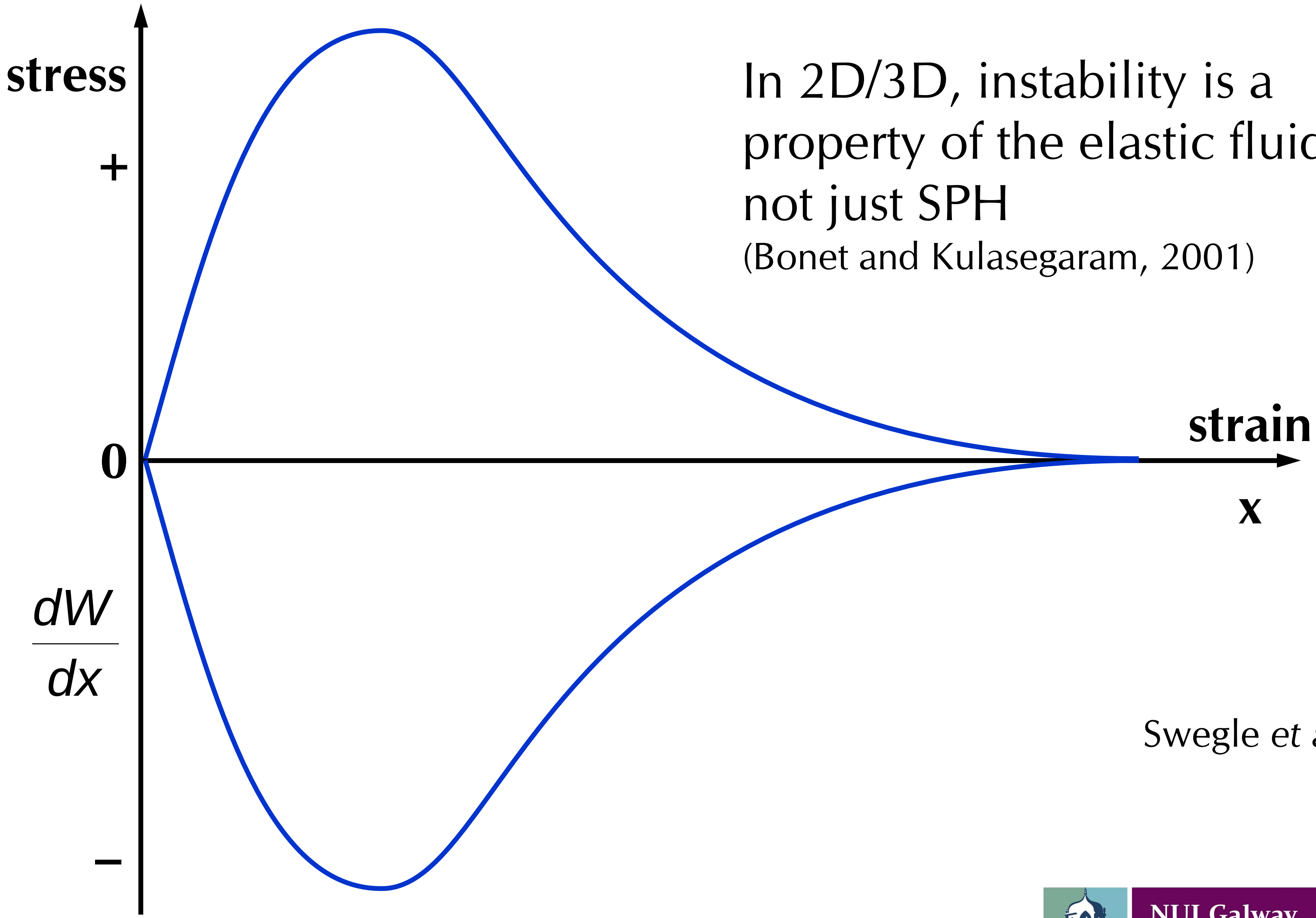
Tensile instability



In 2D/3D, instability is a property of the elastic fluid – not just SPH
(Bonet and Kulasegaram, 2001)

Swegle *et al*. (1995)

Remedies for tensile instability

Repulsive forces (Monaghan, 2000)

- maintain particle distribution
- non-physical momentum source

Total Lagrangian (Rabczuk et al., 2004)

- kernel is a function of material coordinates
- particle retains a constant material coordinate **X** and constant kernel values in **X** space
- suitable for very large deformation (fluids)?

Non-collocational (Dyka and Ingel, 1995)

- stress and velocity stored at different points

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Terminology problems!

Consistency

(1) A consistent discrete approximation to a PDE exactly reproduces the PDE as $\Delta x \rightarrow 0$

(2) A n^{th}-order consistent discrete approximation exactly reproduces n^{th}-order polynomials, always

= completeness, C^n

Consistency: statement of the problem

What is the error in the approximation

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} \cong -\sum_b A\left(x_b\right)\frac{\partial W\left(x_b - x_a\right)}{\partial x_b}\Delta x_b \qquad (1D)$$

?

$$\left.\nabla A\right|_{\mathbf{x}=\mathbf{x}_a} \cong -\sum_b A\left(\mathbf{x}_b\right)\nabla_b W_a V_b \qquad (2D/3D)$$

Methods

Analysis

Taylor series expansions → truncation error in 1D

Numerical Experiments

Evaluation of an analytical test function

for:

- uniform and non-uniform particle distribution
- 1D and 3D
- standard SPH and consistency-corrected kernels

The SPH evaluation of a gradient

Eulerian

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\rho}\nabla p = 0$$

Lagrangian

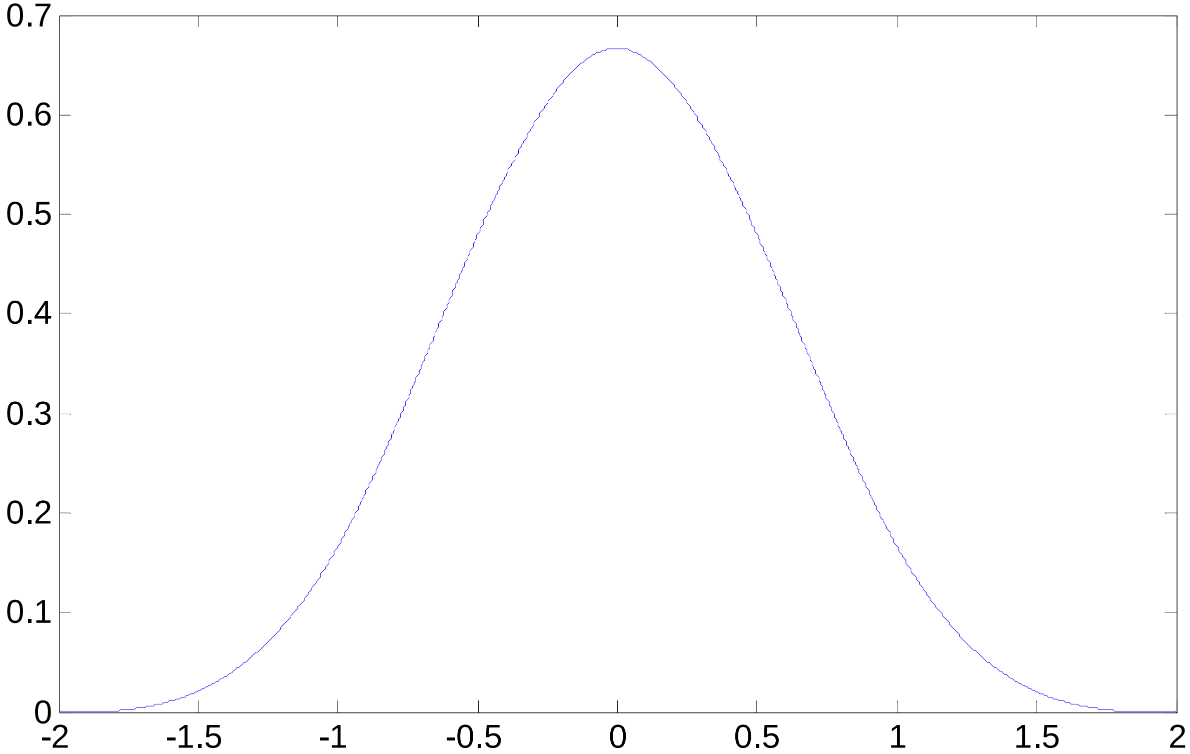
$$\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla p = 0$$

$$\frac{\partial A(x_a)}{\partial x} \cong -\int_{x_a-2h}^{x_a+2h} A(x)\frac{\partial W(x-x_a)}{\partial x}dx \cong -\sum_b A(x_b)\frac{\partial W(x_b-x_a)}{\partial x_b}\Delta x_b$$

smoothing **discretisation**

The dimensionless kernel

$$\hat{W}(s) = hW(x - x_a)$$



$$s = \frac{x - x_a}{h}$$

Smoothing error

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} \cong -\int_{x_a-2h}^{x_a+2h} A \frac{\partial W}{\partial x} dx$$

Expand $A(x)$ as a Taylor series and integrate by parts:

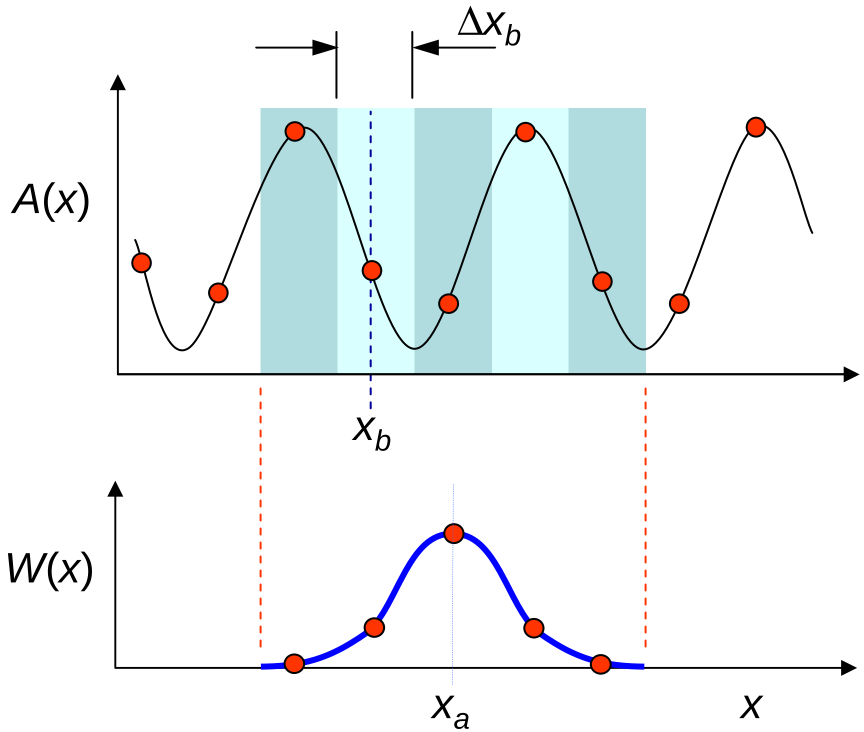
$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} = -\int_{x_a-2h}^{x_a+2h} A \frac{dW}{dx} dx + A'_a \left(1 - \int_{x_a-2h}^{x_i+2h} W dx \right) + \frac{1}{6} \left.\frac{\partial^3 A}{\partial x^3}\right|_a \int_{x_a-2h}^{x_a+2h} (x - x_a)^3 \frac{\partial W}{\partial x} dx + \ldots$$

in dimensionless form:

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} = -\int_{x_a-2h}^{x_a+2h} A \frac{\partial W}{\partial x} dx + A'_a \left(1 - \int \hat{W} ds \right) + \frac{h}{2} A''_a \int s^2 \hat{W}' ds + \frac{h^2}{6} A'''_a \int s^3 \hat{W}' ds + \ldots$$

Discretisation error – special case

- Uniform particle spacing
- $\Delta x/h = 4/n$
- smooth kernel and data



general discretised form:

$$\int_{x_1-\Delta x/2}^{x_n+\Delta x/2} f(x)dx \cong \Delta x \sum_{b=1}^{n} f(x_b)$$

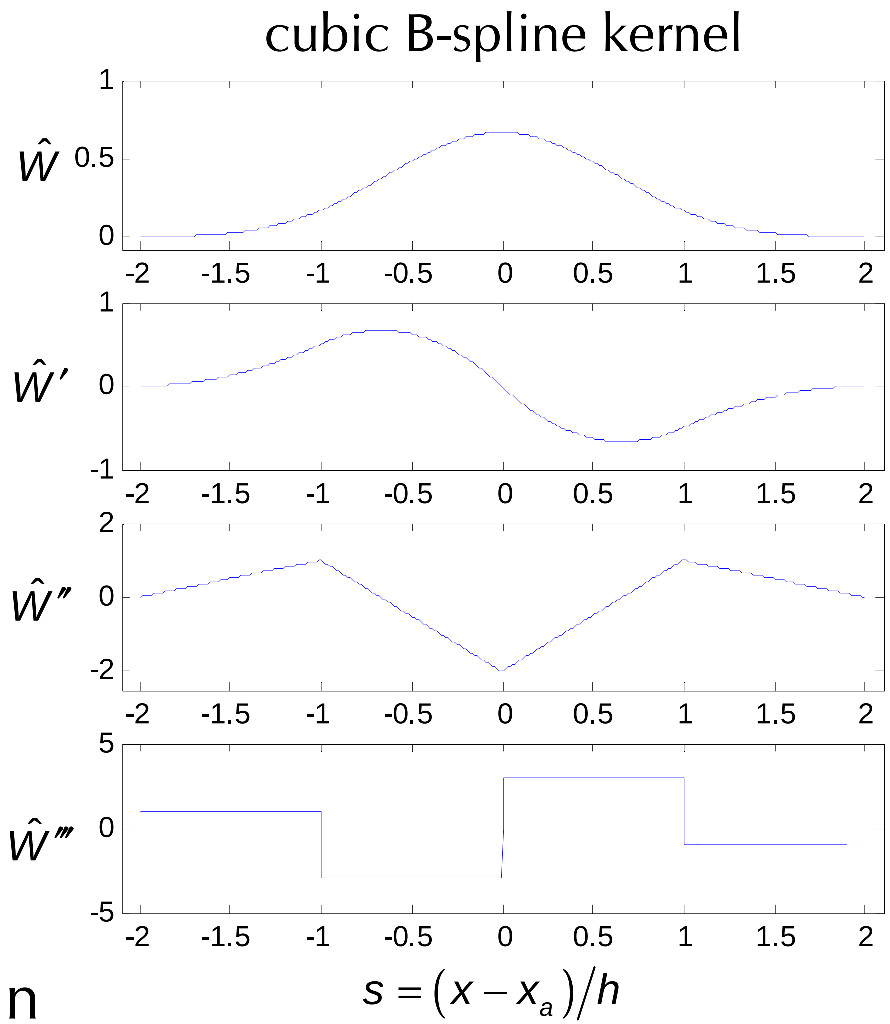
The 2nd Euler-MacLaurin Formula:

$$\int_{x_1-\Delta x/2}^{x_n+\Delta x/2} f(x)dx = \Delta x \sum_{b=1}^{n} f(x_b) - \sum_{k=1}^{\infty} \frac{B_{2k}\Delta x^{2k}}{(2k)!}\left(1-2^{-2k+1}\right)\left(f_{(n+1/2)}^{(2k-1)} - f_{(1/2)}^{(2k-1)}\right)$$

Ralston (1965), Quinlan *et al*. (2005)

Kernel boundary smoothness

Boundary smoothness of the kernel is the highest integer β for which the β^{th} derivative and all lower derivatives are zero at the boundaries of the compact support.



cubic B-spline: $\beta = 2$

Gaussian: $\beta \to \infty$ in infinite domain

polynomial: arbitrary β

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Overall error – uniform particle spacing

SPH estimate

exact derivative

$$-\sum_b A_b W_b' \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

$$+\frac{h^2}{6} A_a''' \int s^3 \hat{W}' ds + \ldots$$

smoothing error

$$-\left(\frac{\Delta x}{h}\right)^{\beta+2} \frac{B_{\beta+2}}{(\beta+2)!}\left(1-2^{-\beta-1}\right)\left[A_a'\left(4\hat{W}_{s=2}^{(\beta+2)}+2(\beta+1)\hat{W}_{s=2}^{(\beta+1)}\right)+O\left(h^2\right)\right]-\ldots$$

discretisation error

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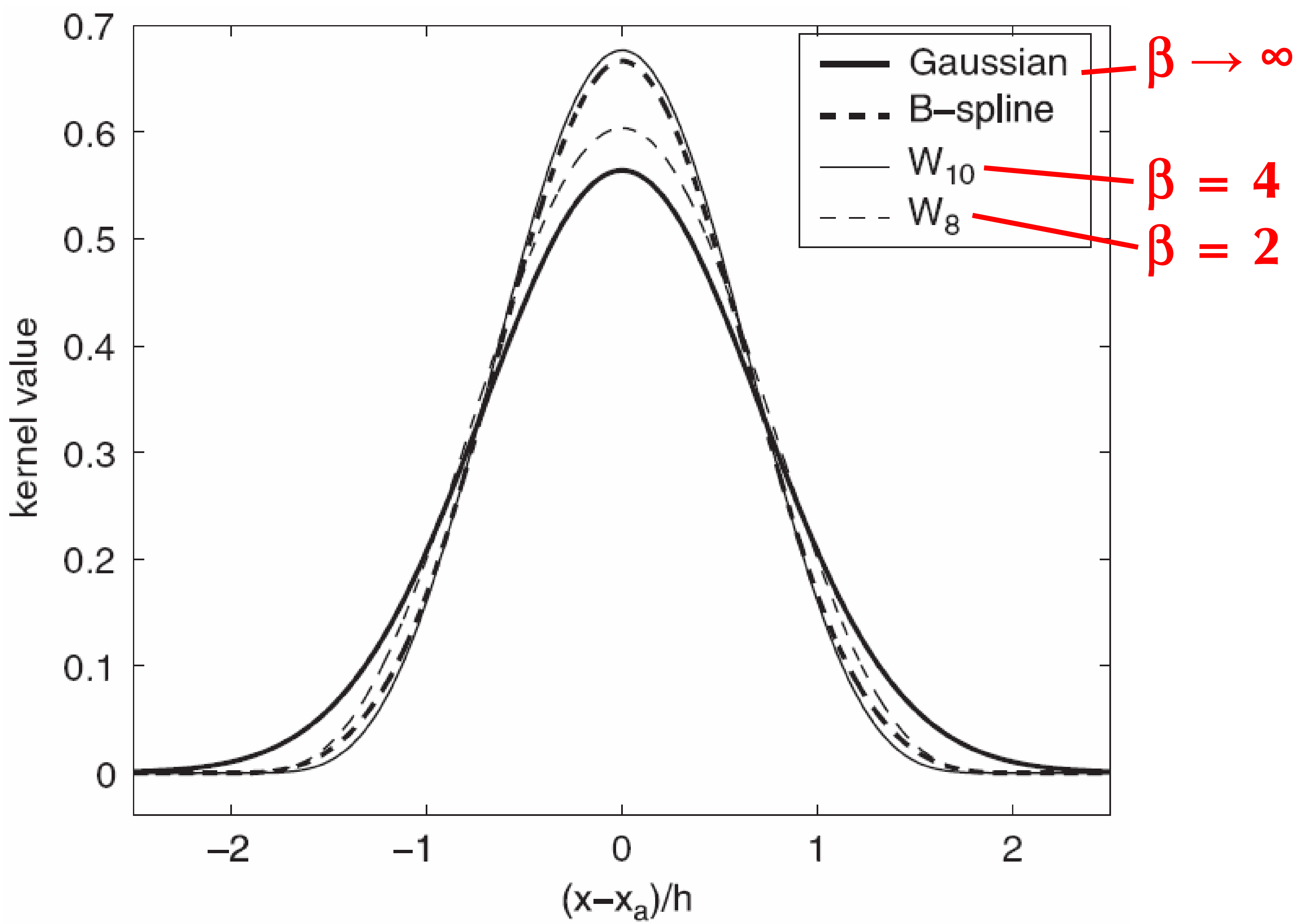
Kernels for testing



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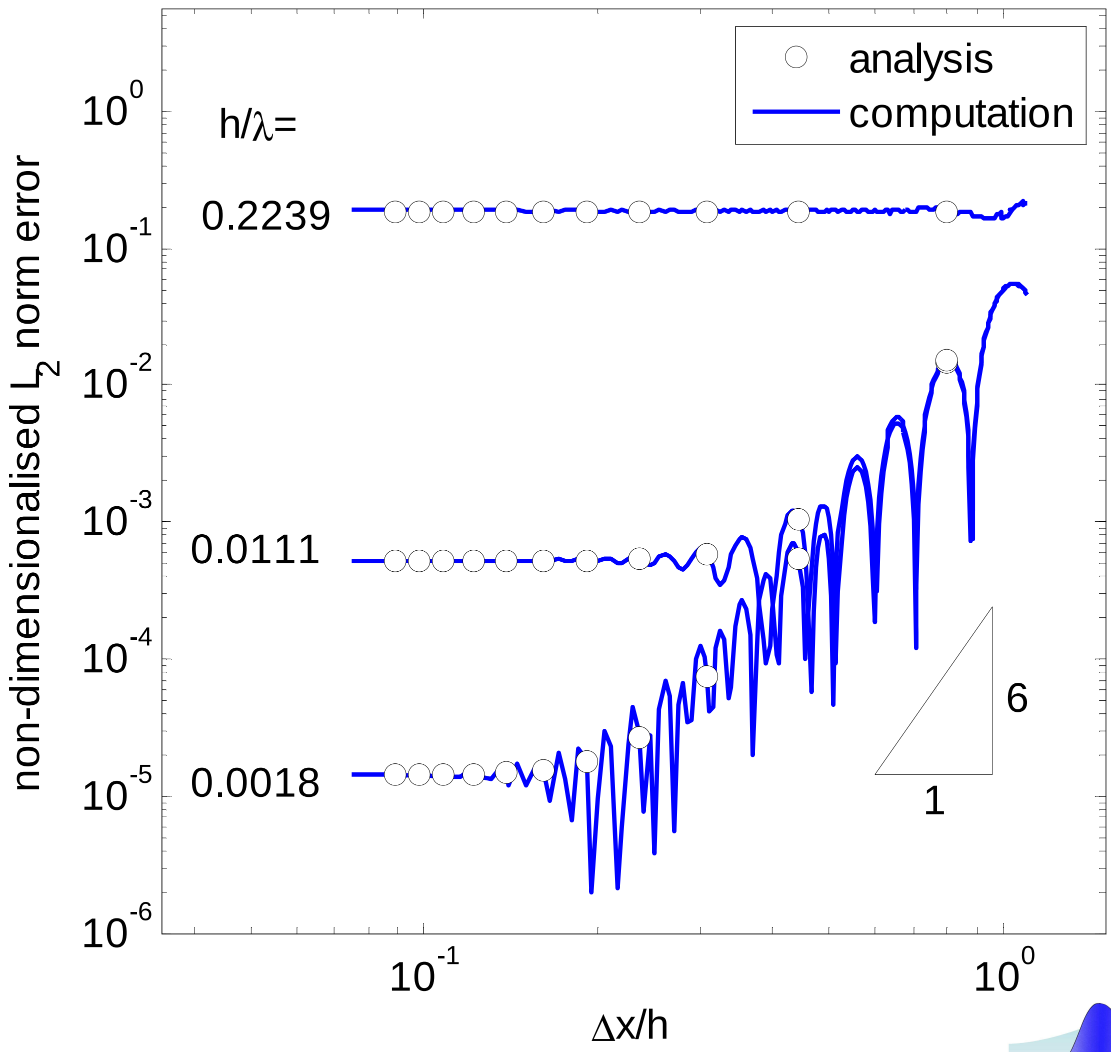
Results – uniform particle spacing, 1D

sinusoidal test function $A(x)$, wavelength λ

10^{th} order polynomial kernel, $\beta = 4$



Results – uniform particle spacing, 1D

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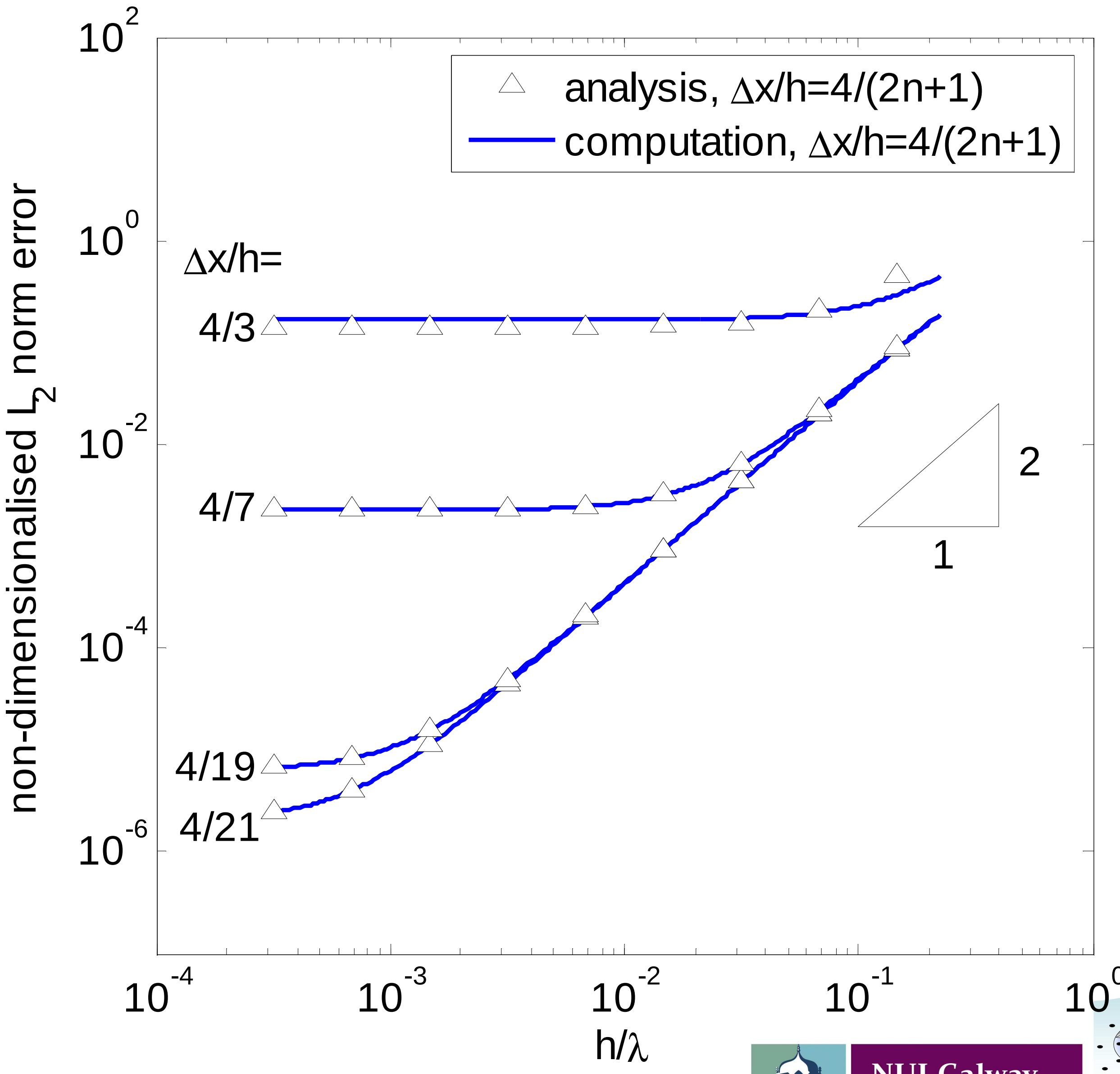

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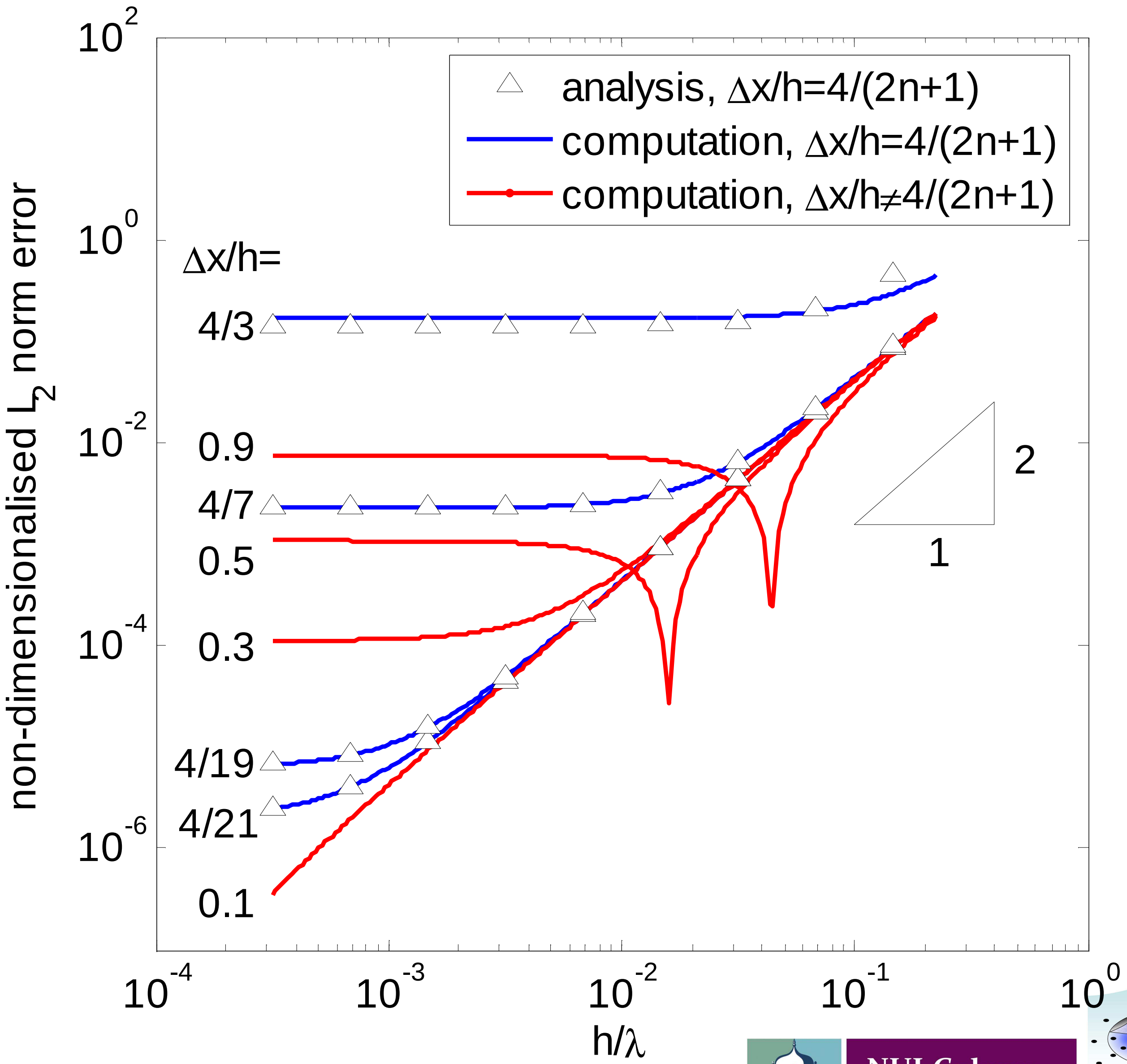
Results – uniform particle spacing, 1D

sinusoidal test function *A*(*x*), wavelength λ

10^{th} order polynomial kernel, $\beta = 4$

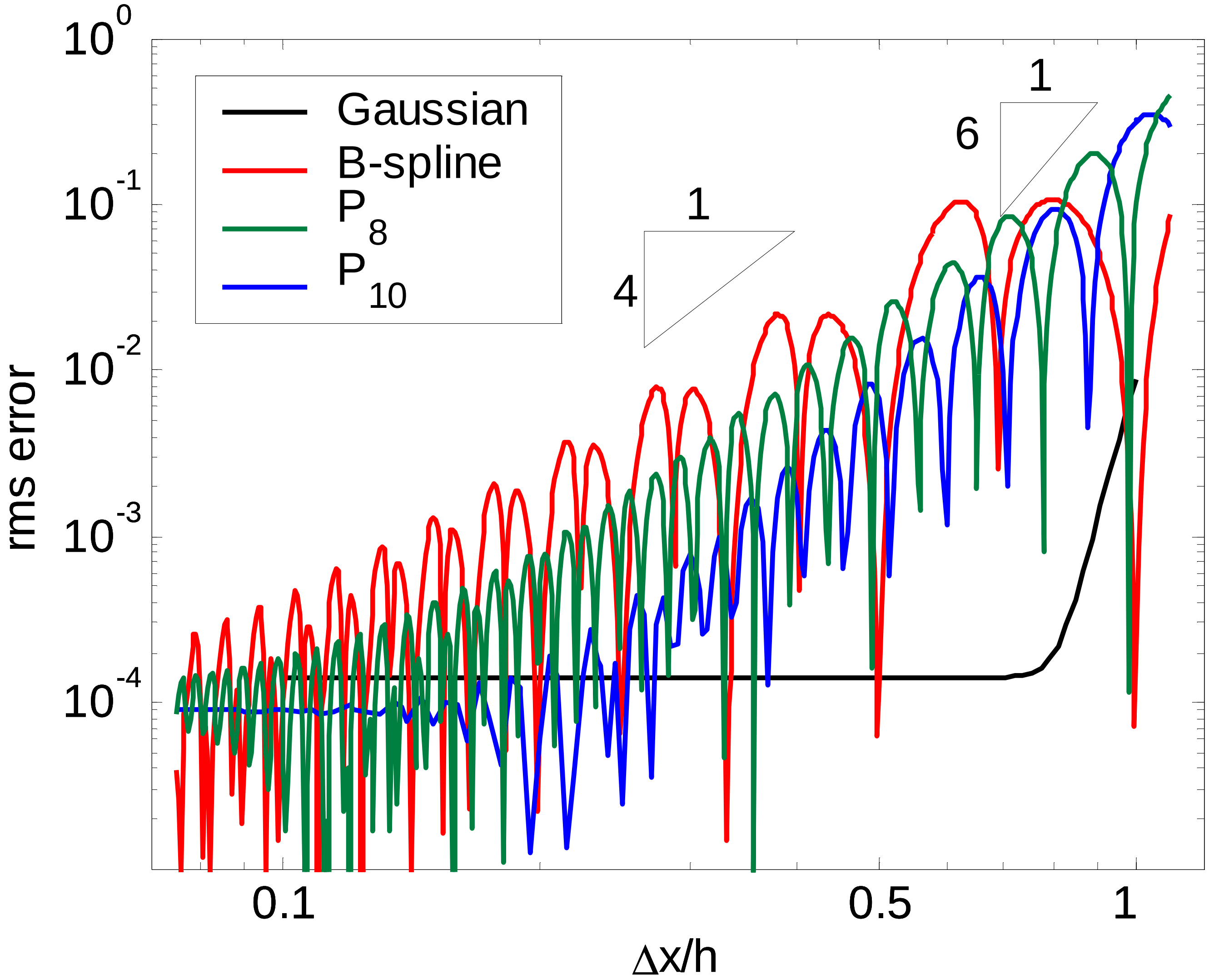


Kernel comparison

Sinusoidal test function, wavelength λ

empirical results

$h/\lambda = 0.0018$



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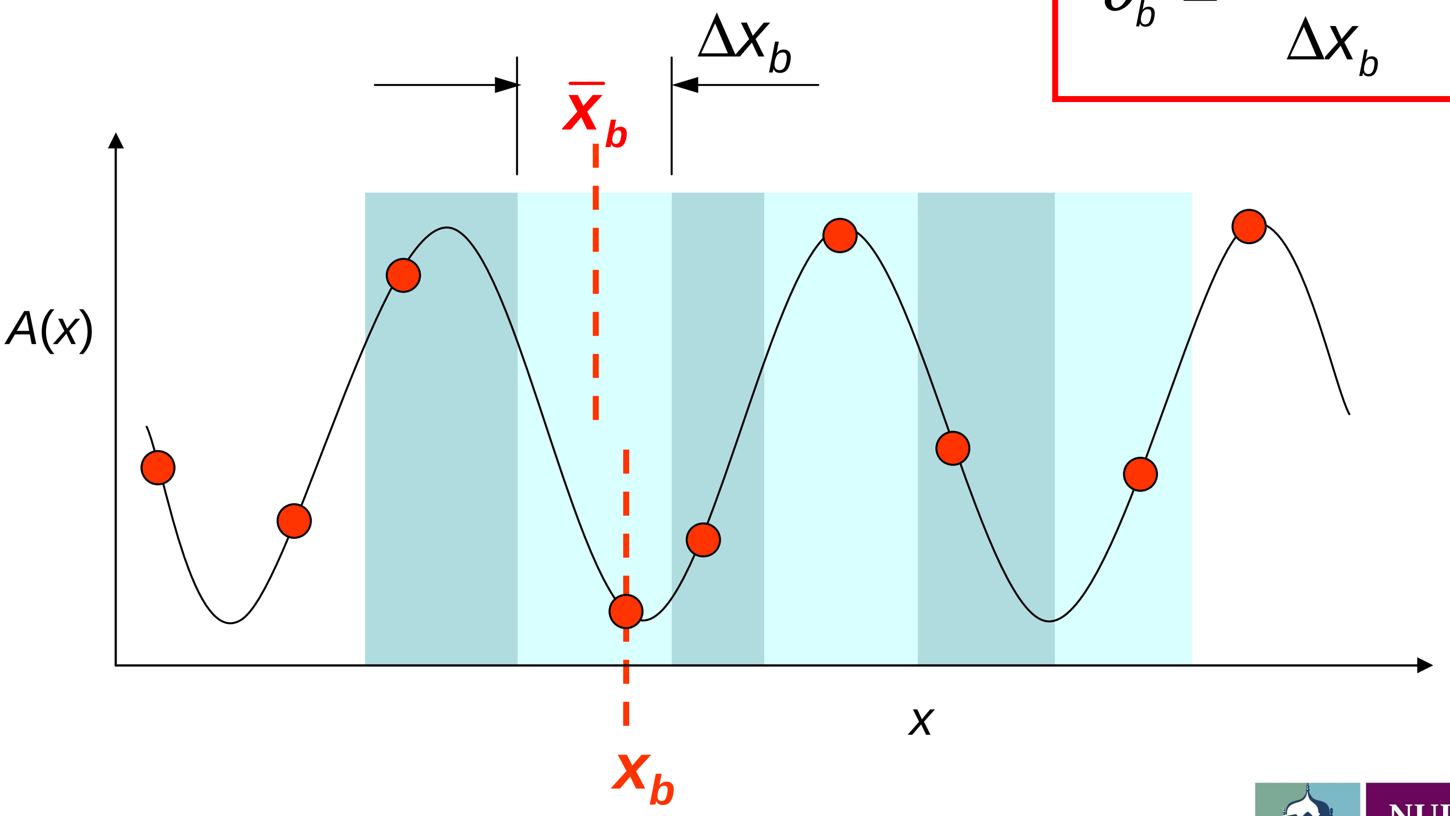
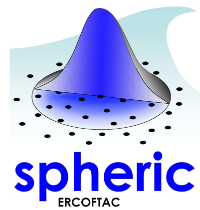
Non-uniform particle distribution

x_b is the location of particle b

$\bar{x}_b$ is the centroid of a region associated with particle b

$$\delta_b = \frac{x_b - \bar{x}_b}{\Delta x_b}$$





Non-uniform spacing

$$-\sum_b A_b W_b' \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

$$-A_a'\left(\int \hat{W} ds - 1\right) + \frac{h^2}{6} A_a''' \int s^3 \hat{W}' ds + \ldots$$ } smoothing error

$$-\frac{1}{h}\left[A_a \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right) + \frac{A_a}{2}\left(\delta^2 + \frac{1}{12}\right) O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right]$$

$$-\left[A_a' \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right)\right]$$

$$-h\left[\frac{A_a''}{2}\delta O\left(\frac{\Delta x}{h}\right) + \frac{A_a''}{2} O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right] - \ldots$$

} discretisation error

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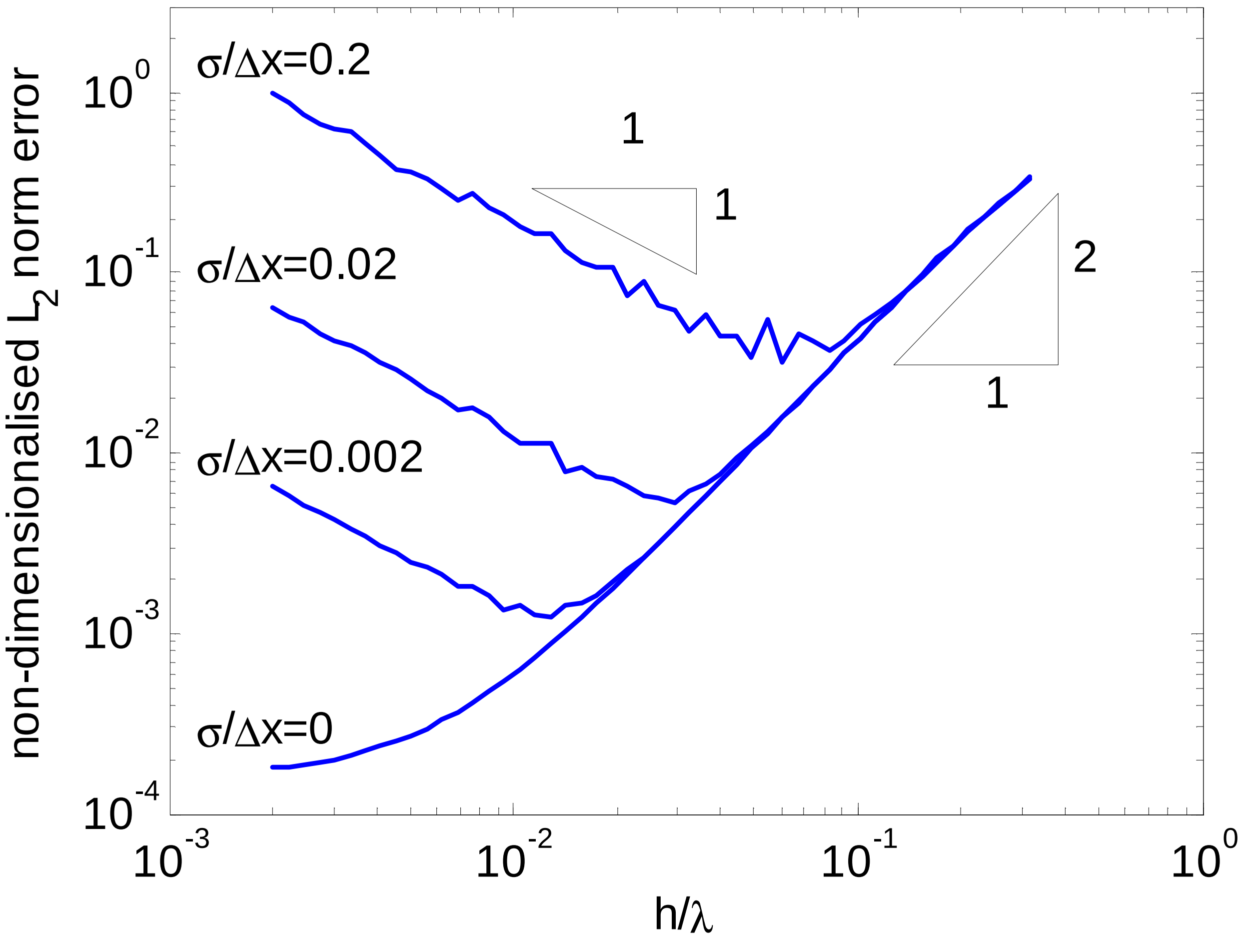
Non-uniform spacing – results

Normally distributed random perturbation of standard deviation σ imposed on uniform particle distribution.

sinusoidal test function, wavelength λ

10^{th} order polynomial kernel, $\beta = 4$

$\Delta x/h = 0.364$



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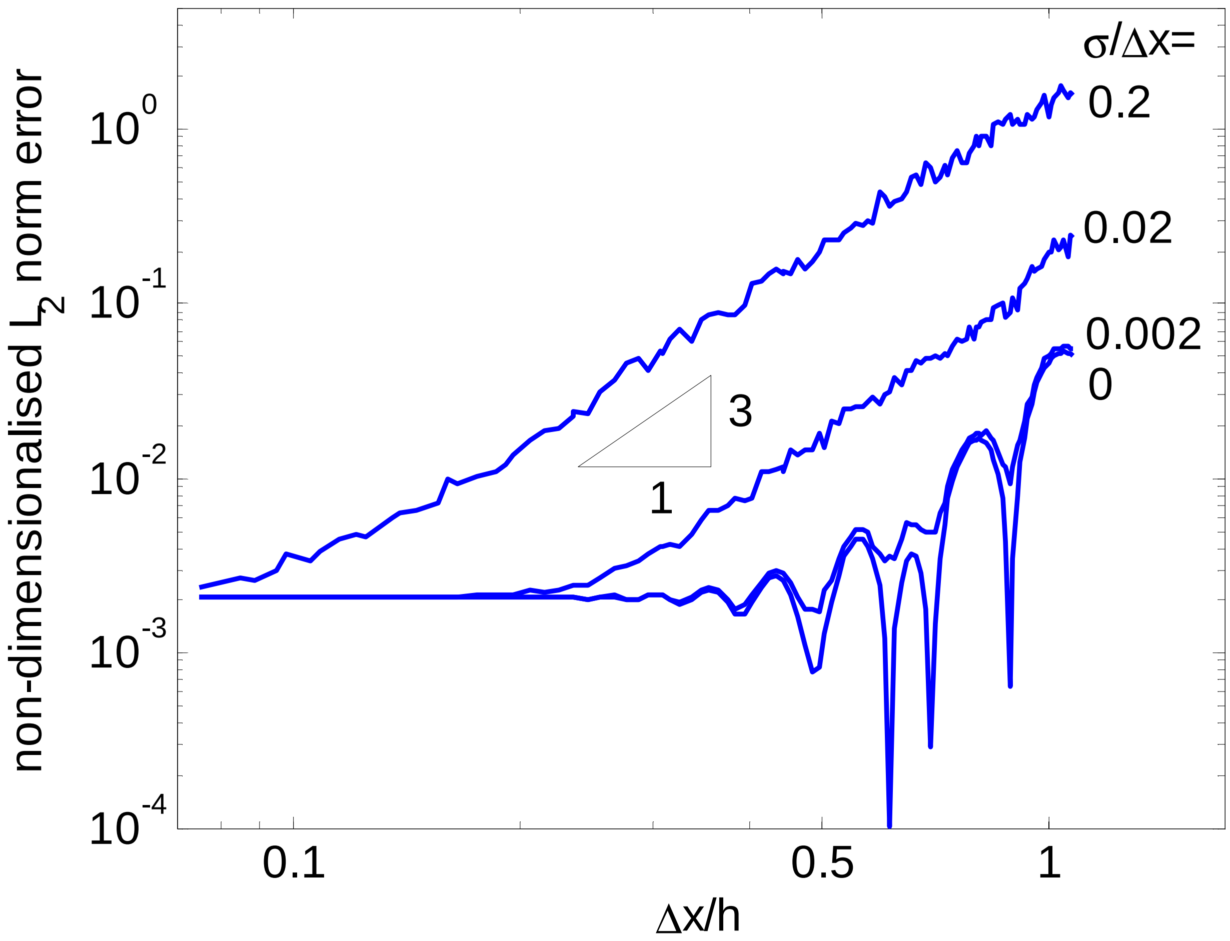
Non-uniform spacing – results

Normally distributed random perturbation of standard deviation **σ** imposed on uniform particle distribution.

sinusoidal test function, wavelength λ

10^{th} order polynomial kernel, $\beta = 4$

$h/\lambda = 0.022$



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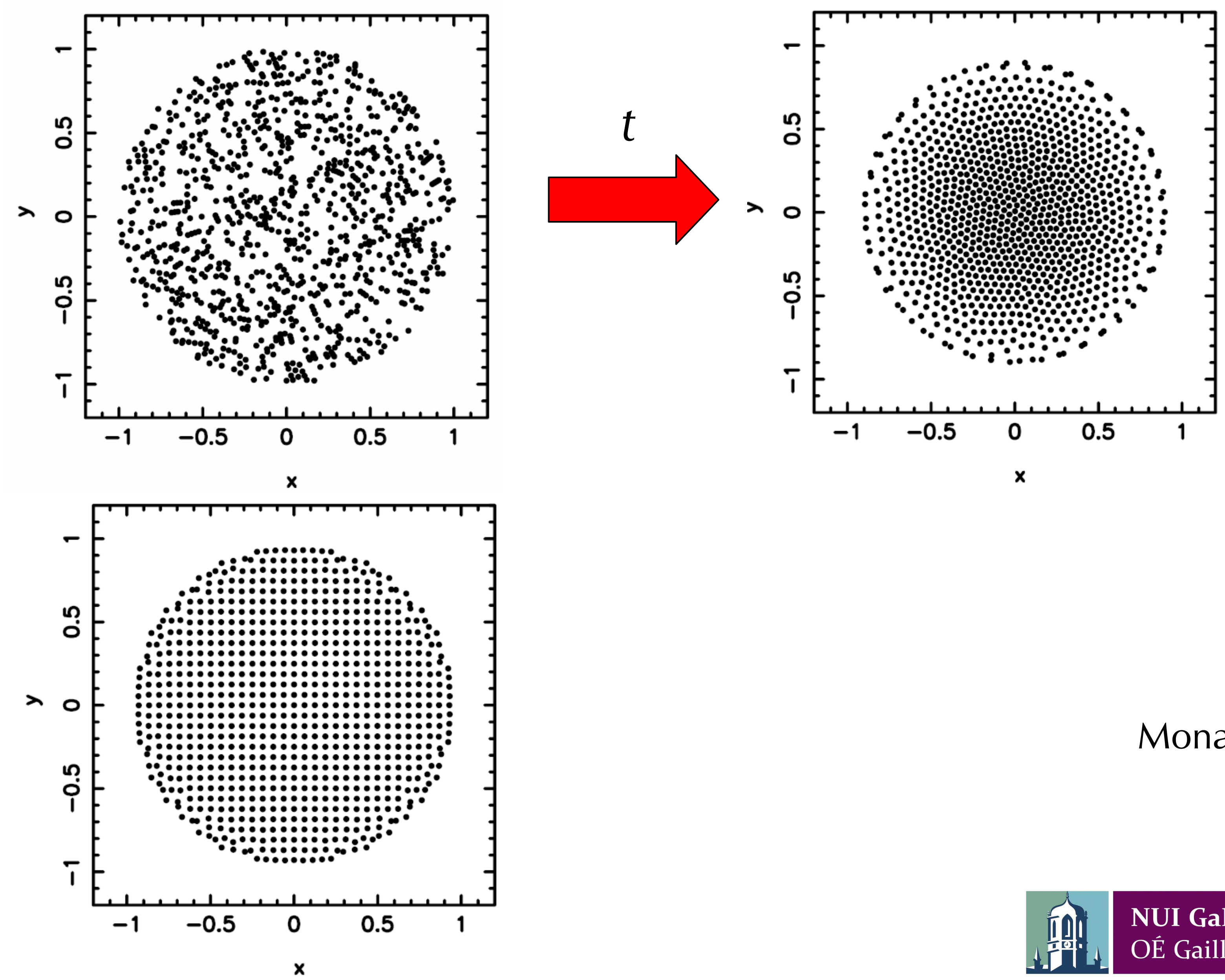
Is randomness a good model for measuring error?



Monaghan (2005)

Is your computer too slow?

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN Vol. 8, No. 6, Nov.—Dec., 1953

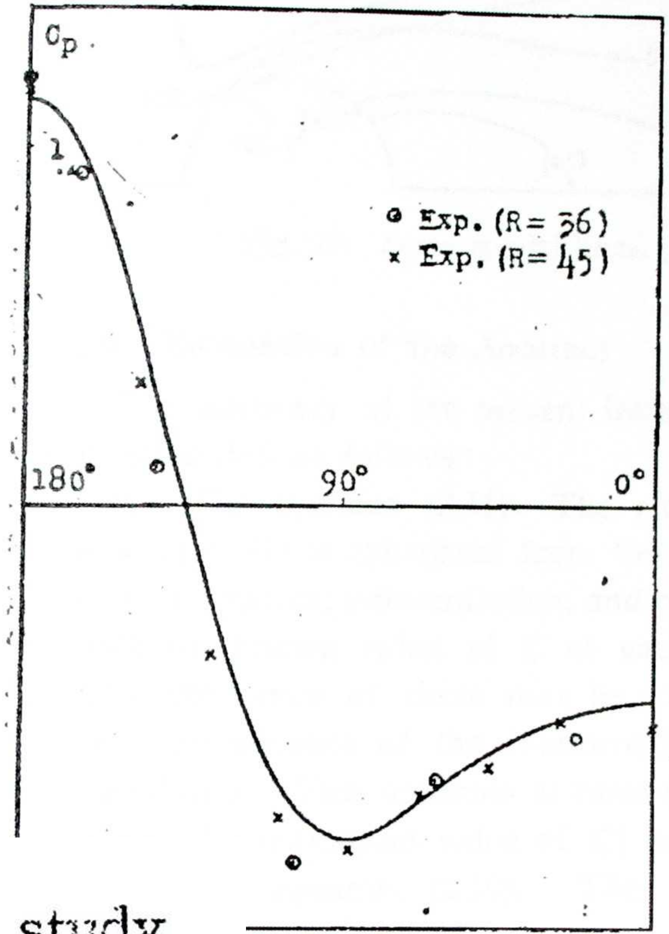
Numerical Solution of the Navier-Stokes Equations for the Flow around a Circular Cylinder at Reynolds Number 40

By Mitutosi KAWAGUTI

Institute of Science and Technology, University of Tokyo

(Received July 10, 1953)

Comparison with Thom's experimental



distribution over the surface.

is made, and the coincidence
good.

The numerical integration in this study took about one year and a half with twenty working hours every week, with a considerable amount of labour and endurance.

Designing kernels for higher orders of consistency

Corrected SPH (CSPH) (Bonet and Lok, 1999; Vignjevic et al., 2000)

$$\tilde{W}\left(\mathbf{x}_b - \mathbf{x}\right) = \frac{W\left(\mathbf{x}_b - \mathbf{x}\right)}{\sum_b W(\mathbf{x}_b - \mathbf{x})V_b}$$

zero-order consistent kernel

$$\left(\sum_b \mathbf{x}_b^T \nabla \tilde{W}(\mathbf{x}_b - \mathbf{x})V_b\right)^{-1} \nabla \tilde{W}$$

first-order consistent kernel gradient

Reproducing Kernel Particle Method (RKPM) (Liu et al., 1995)

$$\sum_b W(\mathbf{x}_b - \mathbf{x})\mathbf{P}\left(\mathbf{x}_b\right)\mathbf{P}\left(\mathbf{x}_b - \mathbf{x}\right)^T \mathbf{c}\left(\mathbf{x}\right) = \mathbf{P}\left(\mathbf{x}\right)$$

$$\tilde{W}(\mathbf{x} - \mathbf{x}_a) = \mathbf{c}\mathbf{P}\left(\mathbf{x}\right)W(\mathbf{x} - \mathbf{x}_a)$$

first-order consistent kernel

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Designing kernels for higher orders of consistency

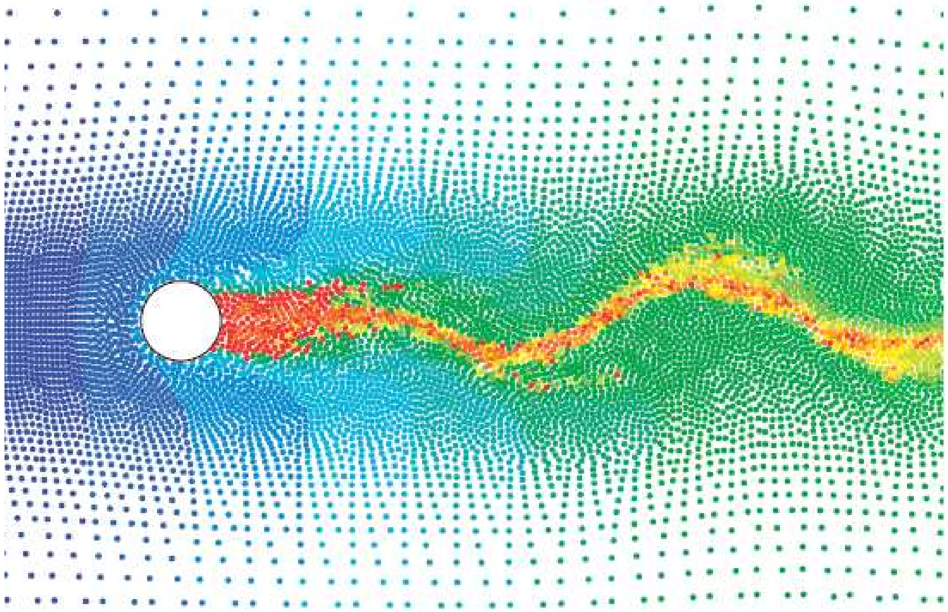
Pro

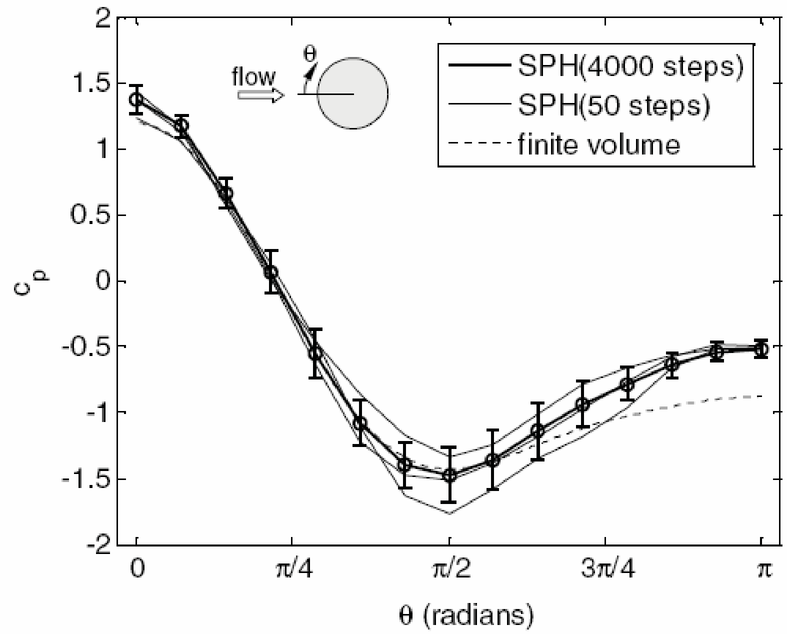
- Better approximations near non-uniform particle distributions
- Better approximations near boundaries
- Less prone to tensile instability? (Bonet and Kulasegaram, 2001)

Con

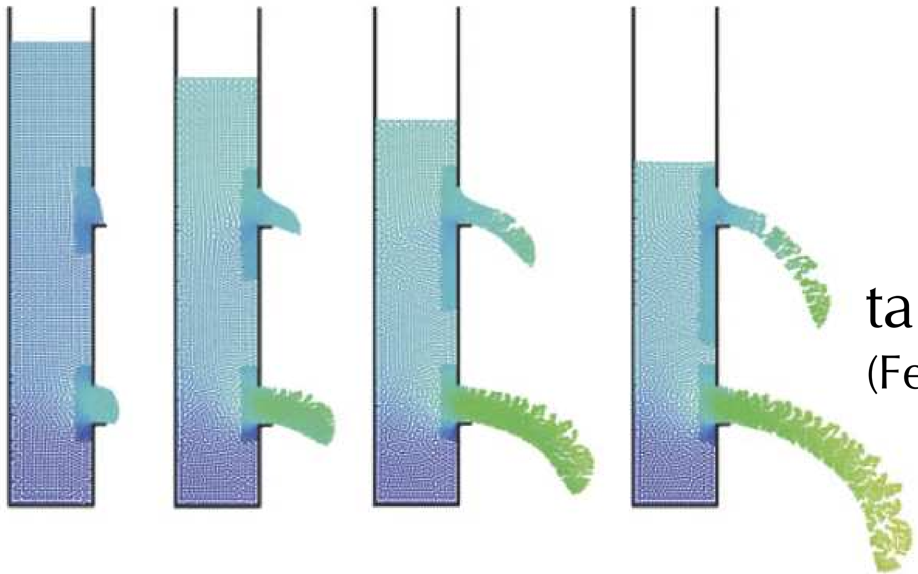
- Corrections must be computed per particle
- Computational effort
- Loss of SPH conservation properties

Consistency-corrected SPH results





cylinder at $Re_d = 100$
(Lastiwka *et al.*, 2008)



tank empyting
(Feldman and Bonet, 2007)

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Truncation error with consistency-corrected kernels

A n^{th}-order consistent kernel ensures exact calculation of gradients of polynomials up to order n.

A general expression for error:

$$\varepsilon = \varepsilon_d + \varepsilon_s = \alpha_0\left(h, \frac{\Delta x}{h}, \delta\right)A_a + \alpha_1\left(h, \frac{\Delta x}{h}, \delta\right)A_a' + \alpha_2\left(h, \frac{\Delta x}{h}, \delta\right)A_a'' + \ldots$$

For a first-order consistent kernel, by definition:

$$\alpha_0 = \alpha_1 = 0$$

Truncation error for first-order consistent kernel

$$-\sum_b A_b W'_b \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

$$-A'_a\left(\int \hat{W} ds - 1\right) + \frac{h}{2} A''_a \int s^2 \hat{W}' ds + \frac{h^2}{6} A'''_a \int s^3 \hat{W}' ds + \ldots \quad \Big\}$$ smoothing error

$$-\frac{1}{h}\left[A_a \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right) + \frac{A_a}{2}\left(\delta^2 + \frac{1}{12}\right) O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right]$$

$$-\left[A'_a \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right)\right]$$

$$-h\left[\frac{A''_a}{2} \delta O\left(\frac{\Delta x}{h}\right) + \frac{A''_a}{2} O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right] - \ldots$$

discretisation error

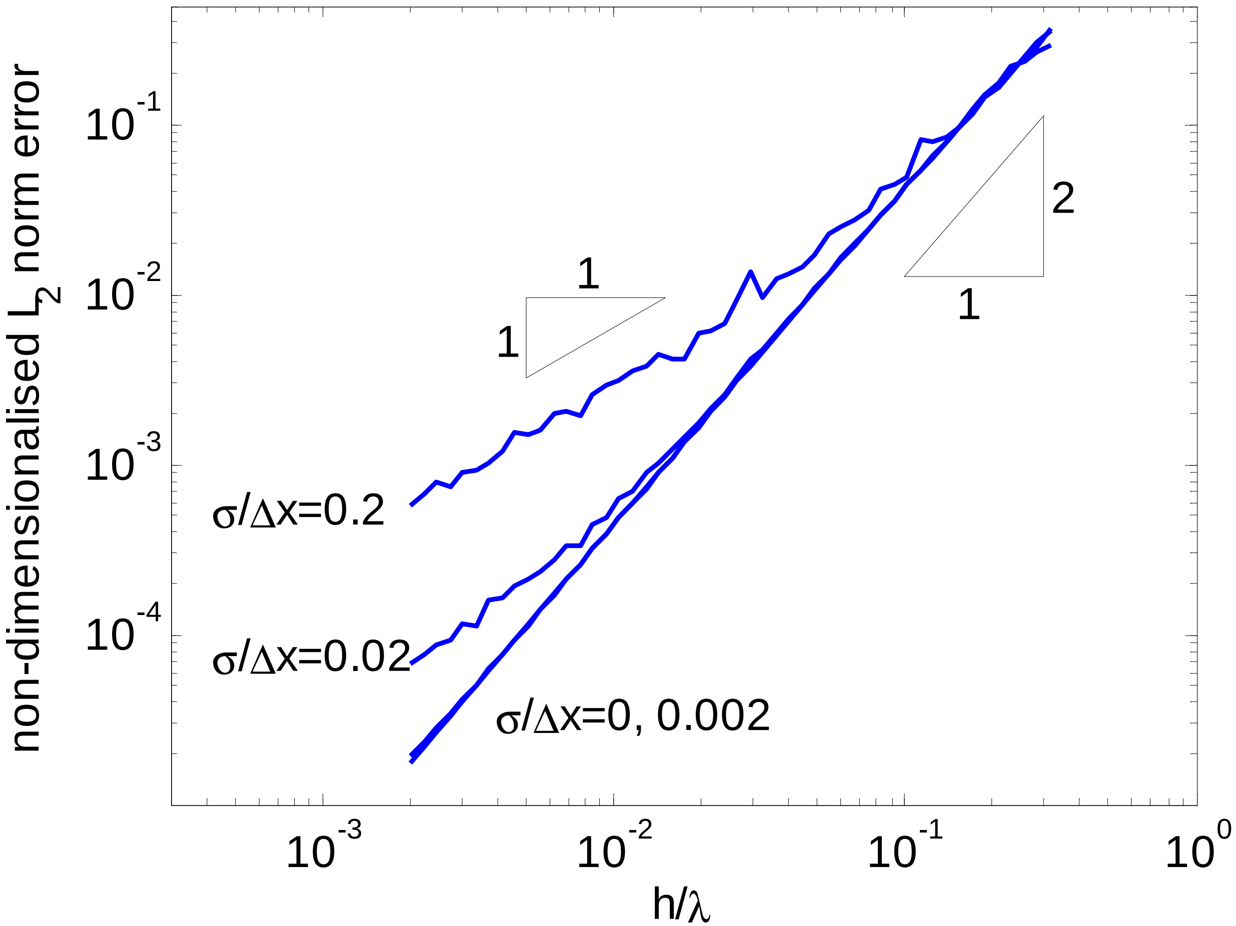
First-order consistent kernel – numerical results

First-order convergence observed in discretisation-limited error

sinusoidal test function, wavelength λ

10th order polynomial kernel, $\beta = 4$

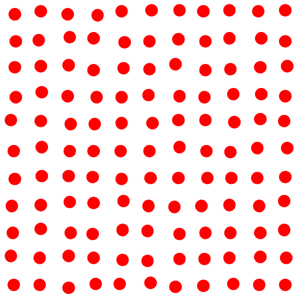
$\Delta x/h = 0.7$

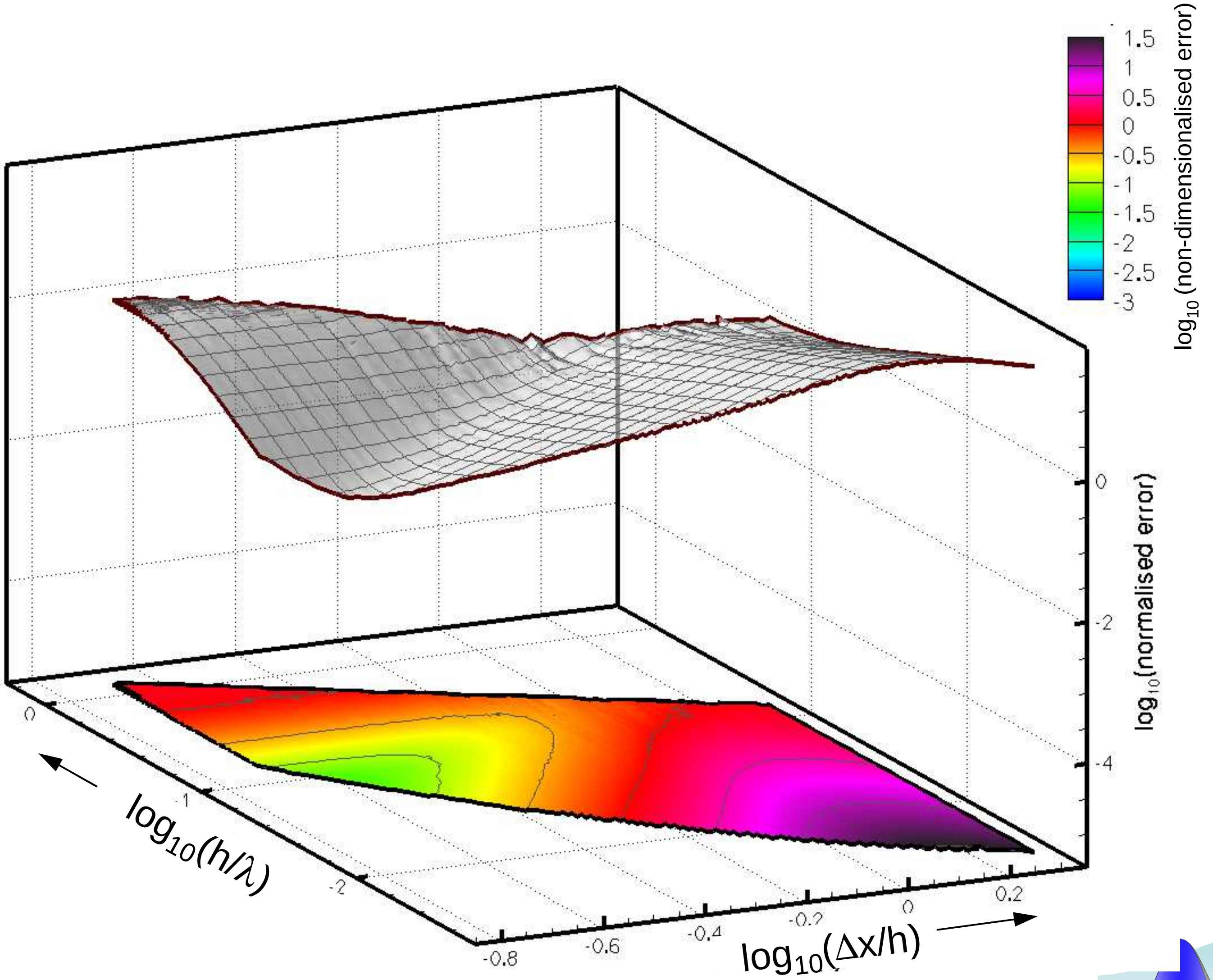


3D standard SPH

$\sigma/\Delta x = 0.2$

(high disorder)





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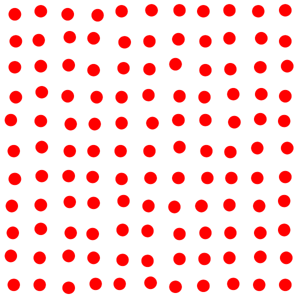
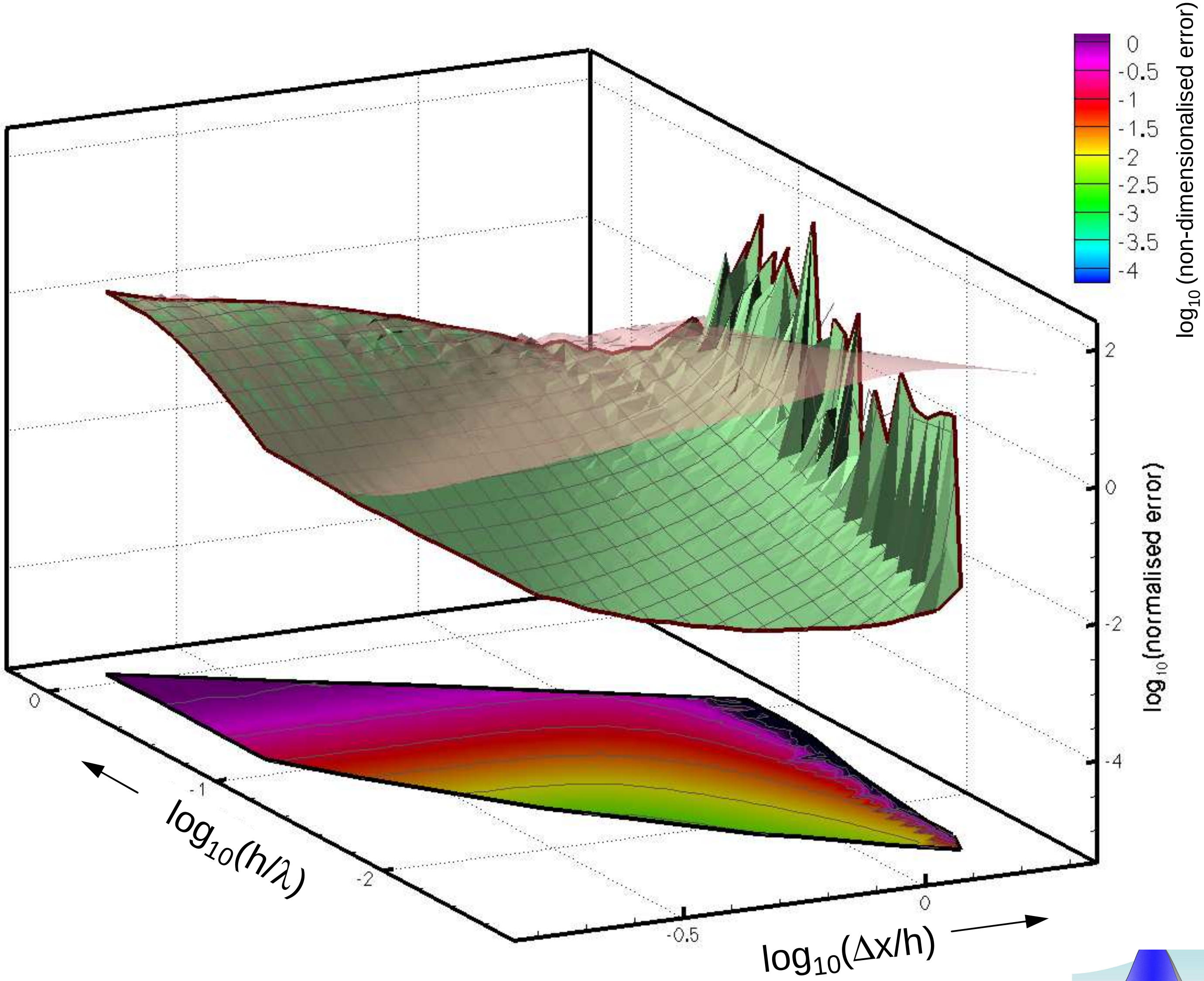
3D standard and corrected SPH

$\sigma/\Delta x = 0.2$

(high disorder)





3D standard SPH

$\sigma/\Delta x = 0.2$

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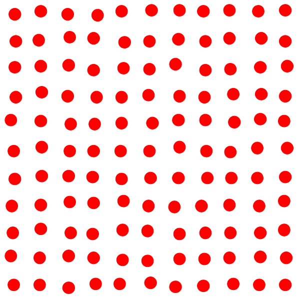

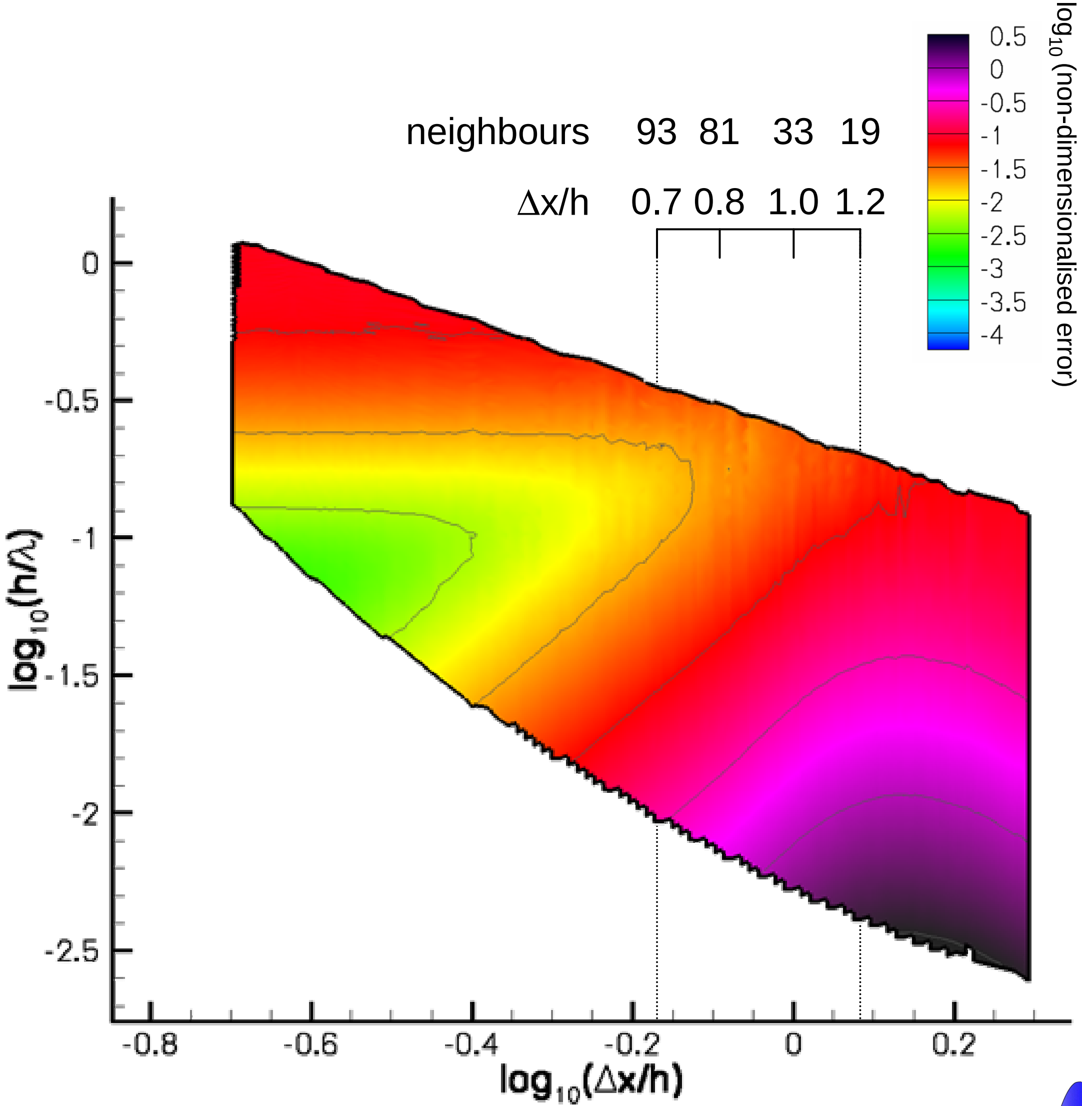

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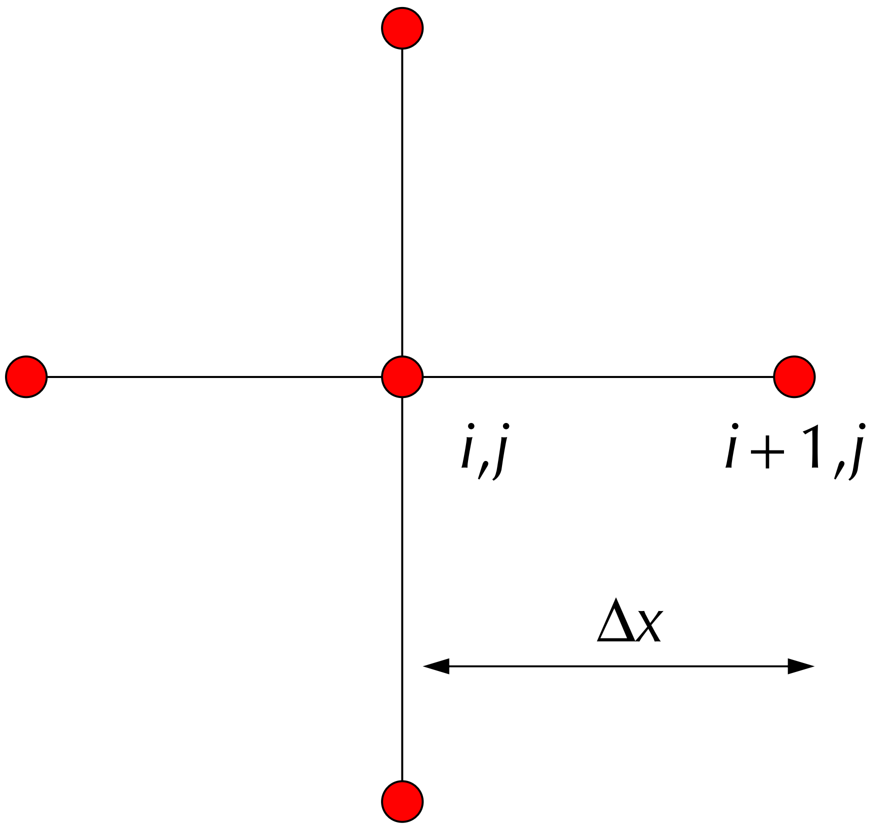
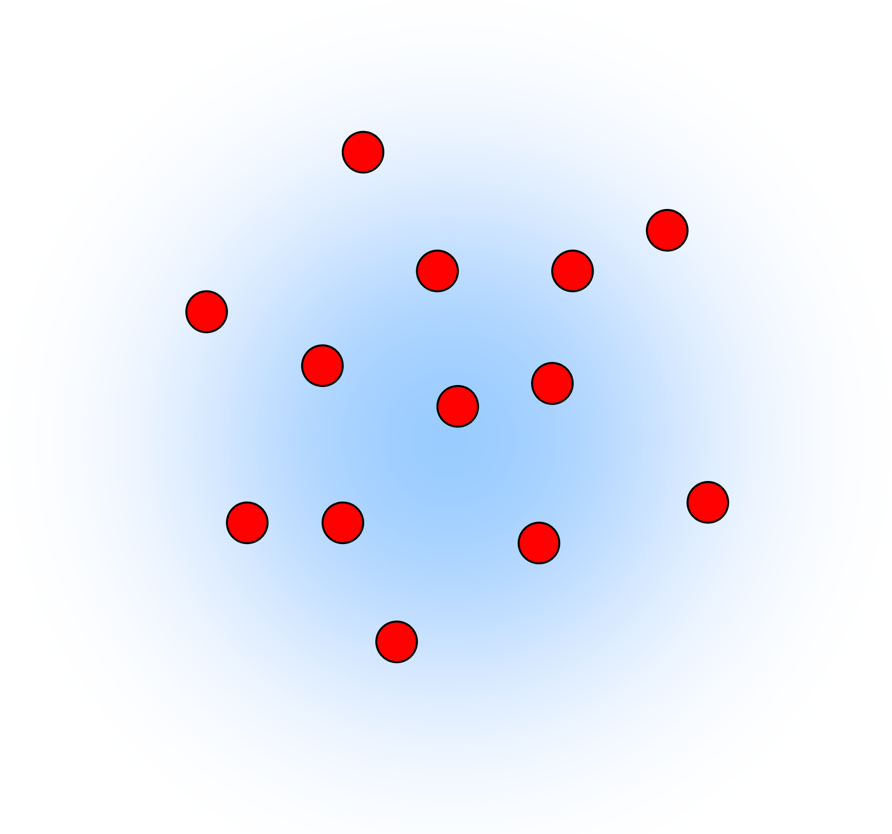
Stencils

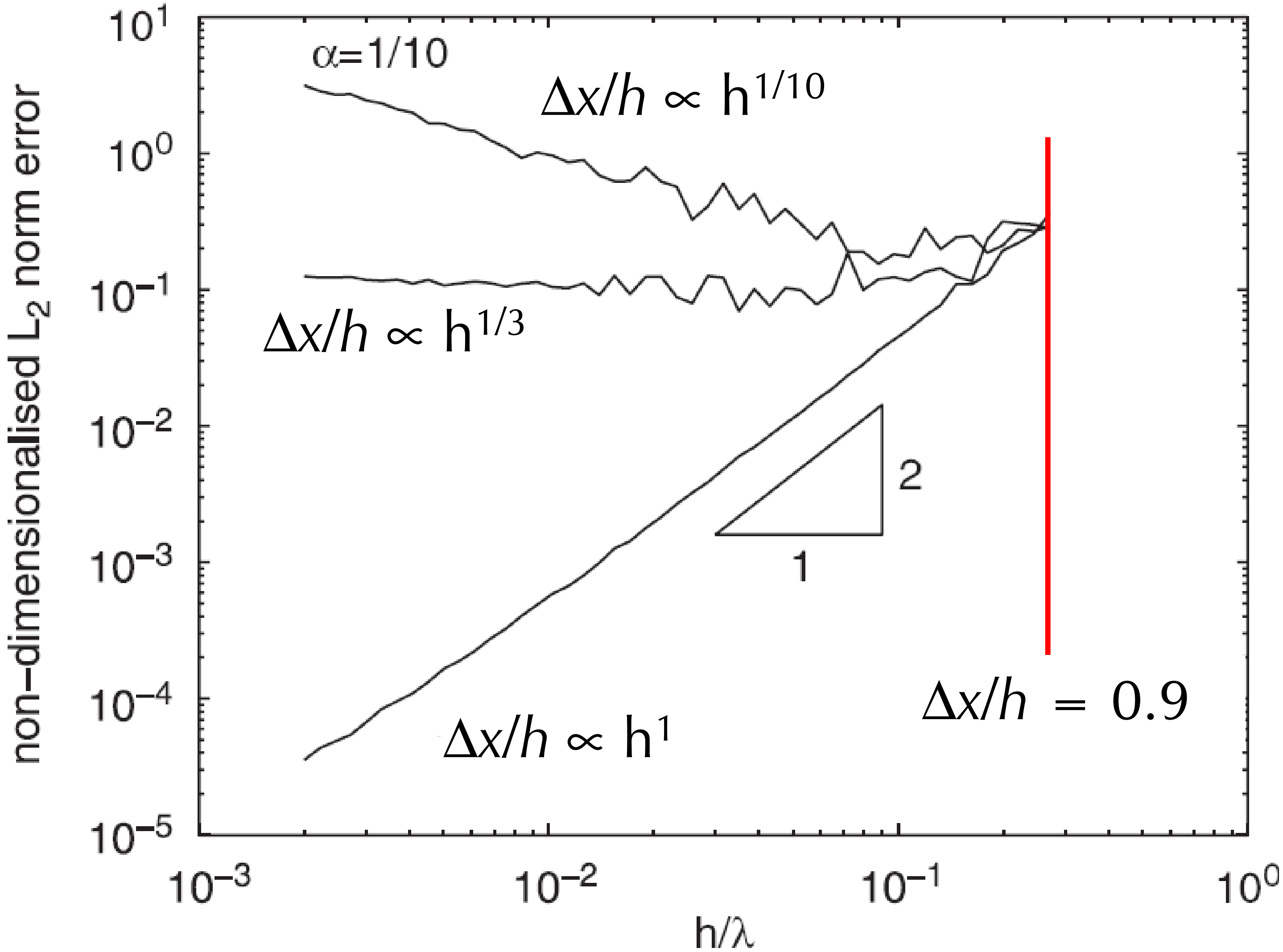


classical finite difference



SPH

Tuning $\Delta x/h$ and h/λ together



Context

Classical "second order" finite difference and finite volume methods are nearly always analysed on uniform meshes. Performance is degraded on non-uniform meshes.

– e.g. Turkel (1986)

"Order of accuracy isn't everything."

– Leveque (2004)

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Second derivatives

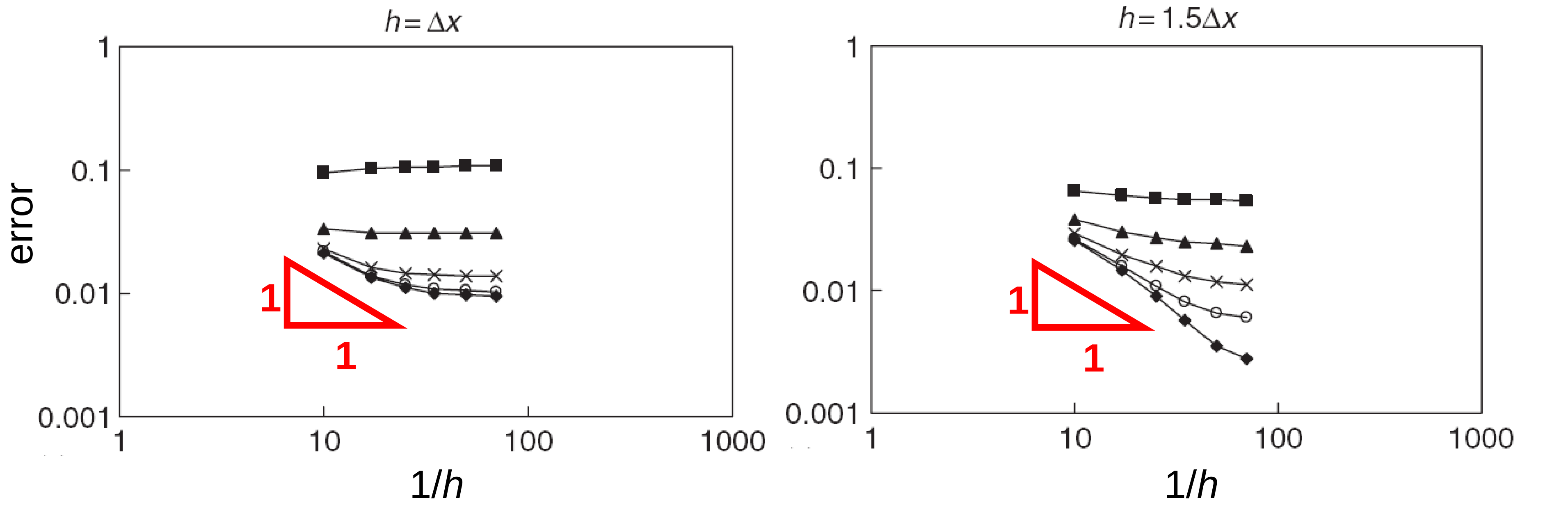
Popular form for computing viscous stress:

$$\nabla^2 A\Big|_a = \sum_b (A_b - A_a) \frac{\mathbf{x}_b - \mathbf{x}_a}{\left|\mathbf{x}_b - \mathbf{x}_a\right|^2} \bullet \nabla W_{ab} \frac{m_b}{\rho_b}$$

Conserves linear and angular momentum

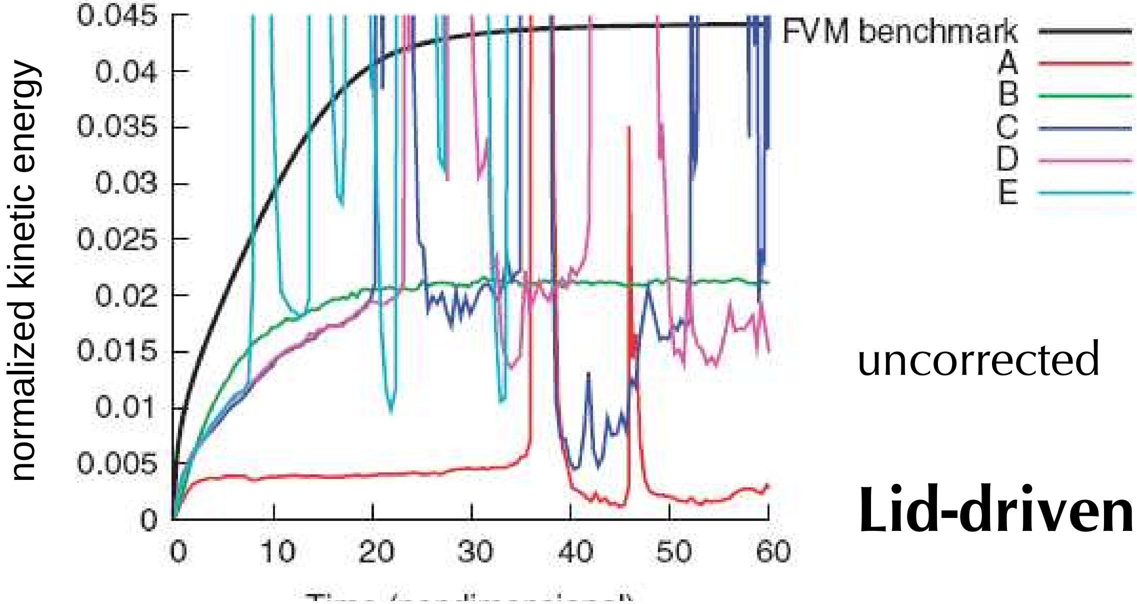
Relies on $(\mathbf{x}_b - \mathbf{x}_a) \parallel \nabla W_{ab}$ – not true for corrected kernels

Error in viscous flow models



Graham and Hughes (2007)

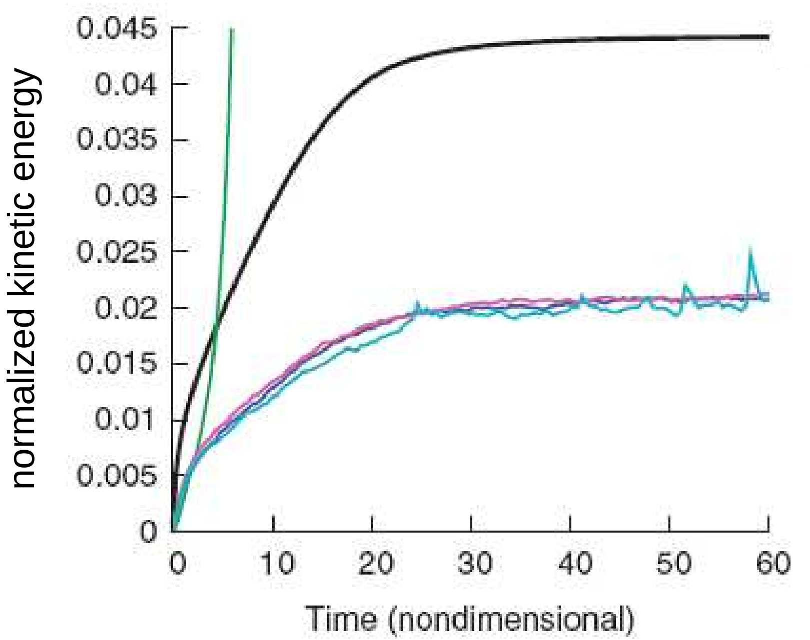
Accuracy of viscous flow models



uncorrected

Lid-driven cavity at $Re_L = 1000$

Basa *et al.* (2008)



first-order consistent

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Conclusions

Convergence requires **consistency**, **conservation**, **stability**

- Difficult to combine conservation and consistency
- Absolute convergence is elusive
- Particle “disorder” is still poorly understood

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