

**FWF National Research Program (NFN)  
Pathways to Habitability (PathH)**

# SPH for simulating impacts and collisions

Thomas I. Maindl  
University of Vienna

Jan 22, 2013

Christoph Schäfer, Roland Speith (Eberhard Karls University of Tübingen)



# Agenda

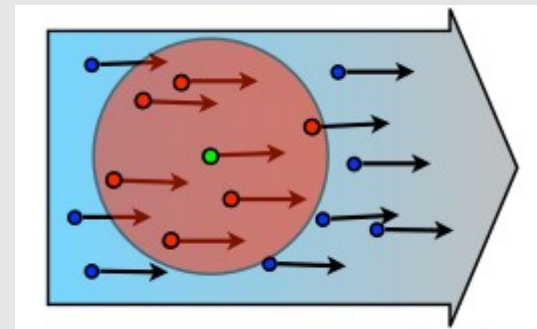
- SPH quick overview
- Solid body physics overview
- Tests and first results
- Outlook
- References

# Smoothed Particle Hydrodynamics (SPH)

- SPH origin: simulating hydrodynamic problems in astrophysics
  - Extended to elasto-plastic dynamics & self gravity
- Application examples include
  - Cosmology
  - Star and planet formation
  - Interactions of stars, black holes,...
  - Accretion discs
  - Material science
  - ...

# SPH is a mesh-free Lagrangian particle method

- Completely different from finite difference and finite volume methods → well suited for comparisons
- The simulated system is represented as a set of interacting “SPH particles” which
  - carry all physical properties of their “fluid part”
  - determine the density in their region (= number of SPH particles in a specific region)
  - move like point masses governed by the Lagrangian form of the equations of motion
  - are to be interpreted as a numerical vehicle rather than physical particles



# SPH principle

- System of coupled PDEs  $\rightarrow$  system of ODEs

## 1. Smooth quantities via kernel convolution

$$f(\mathbf{r}) \longrightarrow \int f(\mathbf{r}') W(|\mathbf{r} - \mathbf{r}'|) d\mathbf{V}' = f(\mathbf{r}) + \mathcal{O}(h^2)$$

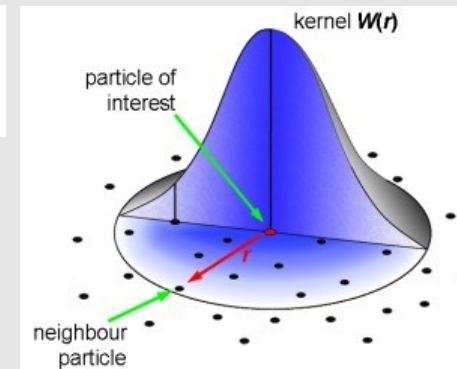
$h$ ... smoothing length, "radius" of kernel, determines spatial resolution

## 2. Remove spatial derivatives

$$\nabla f(\mathbf{r}) \longrightarrow \int f(\mathbf{r}') \nabla W(|\mathbf{r} - \mathbf{r}'|) d\mathbf{V}'$$

## 3. Discretize

$$\nabla f(\mathbf{r}^i) \approx \sum_j \frac{m^j}{\rho^j} f(\mathbf{r}^j) \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h)$$



NUI Galway (2012)

# Example: equivalent formulations

- Equivalent to  $\nabla f(\mathbf{r}^i) \approx \sum_j \frac{m^j}{\rho^j} f(\mathbf{r}^j) \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h)$

to  $\mathcal{O}(h^2)$  ensuring that derivatives of constant functions vanish:

$$\begin{aligned}\nabla f^i &= \frac{\rho^i}{\rho^i} \nabla f^i = \frac{1}{\rho^i} [\nabla(\rho^i f^i) - f^i \nabla \rho^i] \\ &\approx \frac{1}{\rho^i} \sum_j \frac{m^j}{\rho^j} \rho^j f^j \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h) - \frac{f^i}{\rho^i} \sum_j \frac{m^j}{\rho^j} \rho^j \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h) \\ &= \frac{1}{\rho^i} \sum_j m^j (f^j - f^i) \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h)\end{aligned}$$

# Problem-dependent equation formulation

- Example Euler equation

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla p \quad \frac{d\mathbf{v}^i}{dt} = -\sum_j \frac{m^j p^j}{\rho^j \rho^i} \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h)$$

- Equivalent to  $\mathcal{O}(h^2)$  and numerically more stable:

$$\frac{d\mathbf{v}^i}{dt} = -\sum_j m^j \frac{p^i + p^j}{\rho^i \rho^j} \nabla W(|\mathbf{r}^i - \mathbf{r}^j|, h)$$

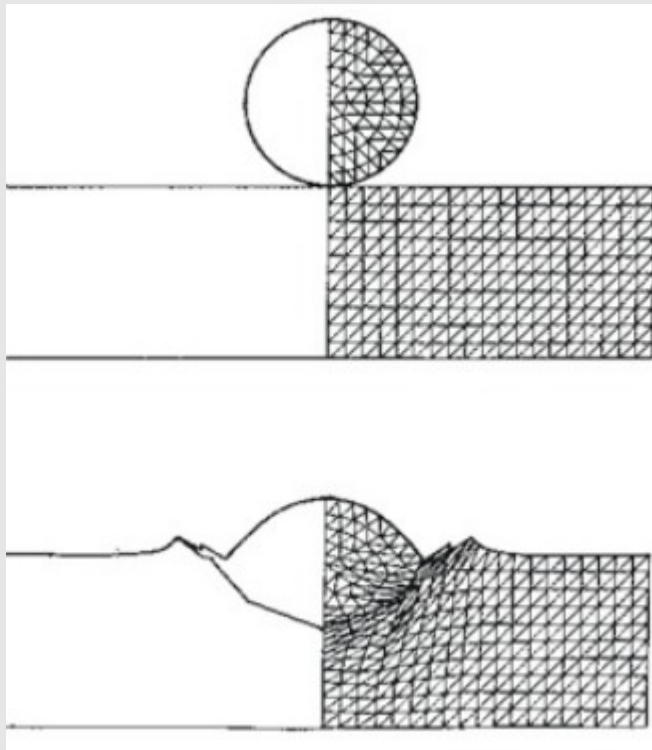
- using  $\lambda=1$  in the identity

$$\frac{1}{\rho^{2-\lambda}} \nabla \frac{p}{\rho^{\lambda-1}} = \frac{1}{\rho} \nabla p - \frac{p}{\rho^\lambda} \nabla \rho^{\lambda-1}$$

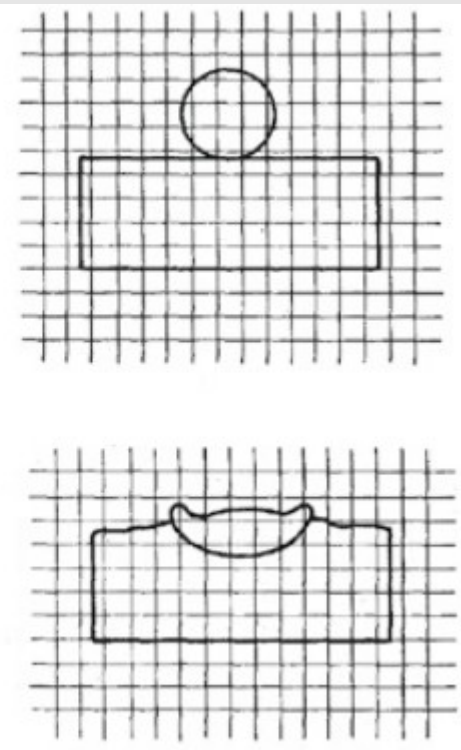
# SPH for impact simulations

Mesh-free Lagrangian method provides natural reference frame for treating deformations and fragmentation

Lagrange scheme



Euler scheme

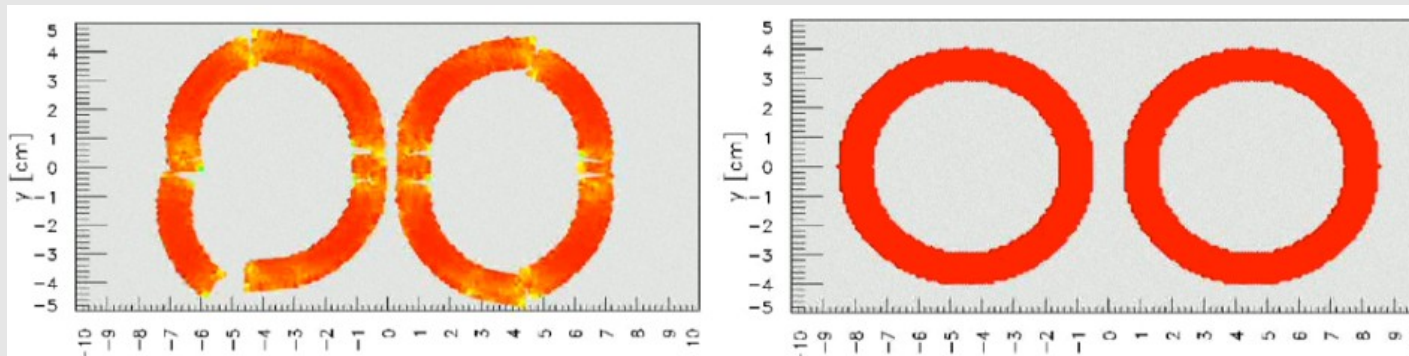


Lagrange scheme: number of “grid points” resolving the object is not reduced by deformation



# Special SPH topics

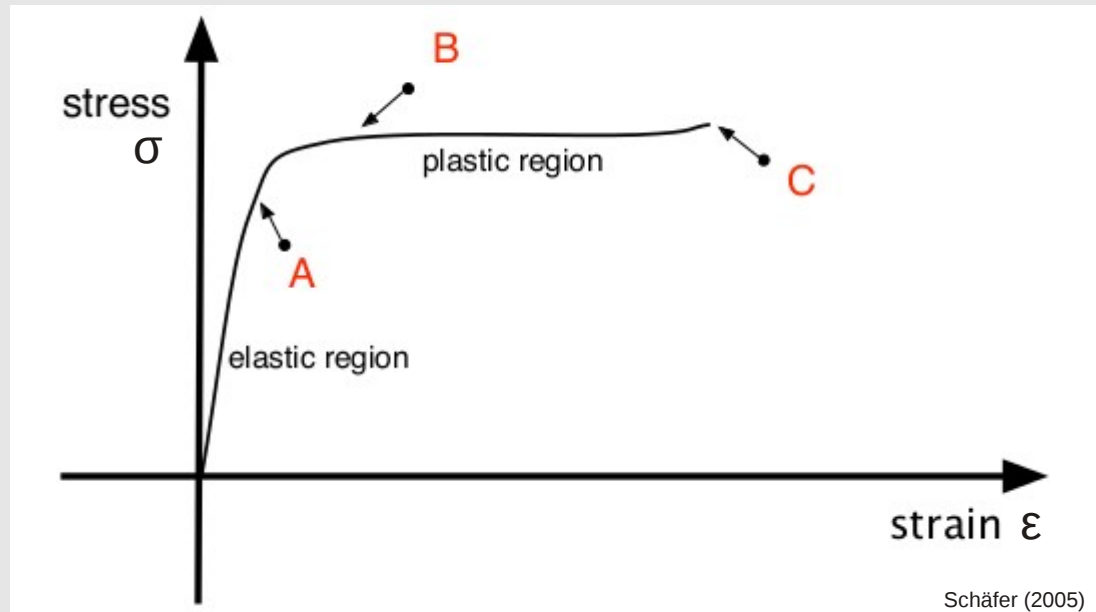
- Tensile instability
  - Artificial clumping leading to unphysical results



Speith (2012)

- Solution: small artificial repulsive stress (Monaghan 2000)
- There are other SPH issues
  - XSPH
    - Smooth velocities preventing mutual penetration
  - Artificial viscosity
    - Prevents mutual penetration of particles
  - Integrate density rather than using  $\rho = \sum m W$  for stable surfaces
  - ...

# Solid bodies: continuum mechanics



- A) Hooke's law: elasticity, deviatoric stress rate proportional to strain rate
- B) Yielding relations: plasticity by modifying stresses beyond the elastic limit
- C) Damage model and brittle failure for tensile stresses beyond material strength

# Material equations

Continuity equation (mass conservation):

$$\frac{d\rho}{dt} = -\rho \frac{\partial v^\alpha}{\partial x^\alpha}$$

EOM (conservation of momentum):

$$\frac{dv^\alpha}{dt} = \frac{1}{\rho} \frac{\partial \sigma^{\alpha\beta}}{\partial x^\beta} - \frac{\partial \Phi}{\partial x^\alpha}, \quad \text{stress tensor } \sigma^{\alpha\beta} = -p \delta^{\alpha\beta} + S^{\alpha\beta}$$

Energy conservation:

$$\frac{du}{dt} = -\frac{p}{\rho} \frac{\partial v^\alpha}{\partial x^\alpha} + \frac{1}{\rho} S^{\alpha\beta} \dot{\epsilon}^{\alpha\beta}, \quad \text{strain rate tensor } \dot{\epsilon}^{\alpha\beta} = \frac{1}{2} \left( \frac{\partial v^\alpha}{\partial x^\beta} + \frac{\partial v^\beta}{\partial x^\alpha} \right)$$

Constitutive equation:

$$\frac{dS^{\alpha\beta}}{dt} = 2\mu \left( \dot{\epsilon}^{\alpha\beta} - \frac{1}{3} \delta^{\alpha\beta} \dot{\epsilon}^{\gamma\gamma} \right) + S^{\alpha\gamma} R^{\gamma\beta} + S^{\beta\gamma} R^{\gamma\alpha}$$

with rotation rate tensor  $R^{\alpha\beta} = \frac{1}{2} \left( \frac{\partial v^\alpha}{\partial x^\beta} - \frac{\partial v^\beta}{\partial x^\alpha} \right)$

EOS:  $p = p(\rho, u)$

# Plastic behavior: von Mises yielding criterion

Limit deviatoric stress tensor by

$$S^{\alpha\beta} = f S^{\alpha\beta}$$

with

$$f = \min \left[ \frac{Y_0^2}{3 J_2}, 1 \right], \quad J_2 = \frac{1}{2} S^{\alpha\beta} S^{\alpha\beta}$$

and the material dependent yield stress  $Y_0$

# Equation of state

- Connects the thermodynamic variables  $\rho$ ,  $p$ , and  $u$  to close the set of equations
- Several analytical and semi-empirical approaches exist, e.g.,

- Murnaghan EOS (isothermal only)

$$p = \frac{K_0}{n} \left[ \left( \frac{\rho}{\rho_0} \right)^n - 1 \right]$$

- Tillotson (1962) EOS

$$p = \left( a + \frac{b}{\frac{u}{u_0 \eta^2} + 1} \right) \rho u + A\mu + B\mu^2, \quad \eta = \frac{\rho}{\rho_0}, \quad \mu = \eta - 1 \quad (u < u_{iv})$$

$$p = a\rho u + \left[ \frac{b\rho u}{\frac{u}{u_0 \eta^2} + 1} + A\mu e^{-\beta(\frac{\rho_0}{\rho} - 1)} \right] e^{-\alpha(\frac{\rho_0}{\rho} - 1)} \quad (u > u_{cv})$$

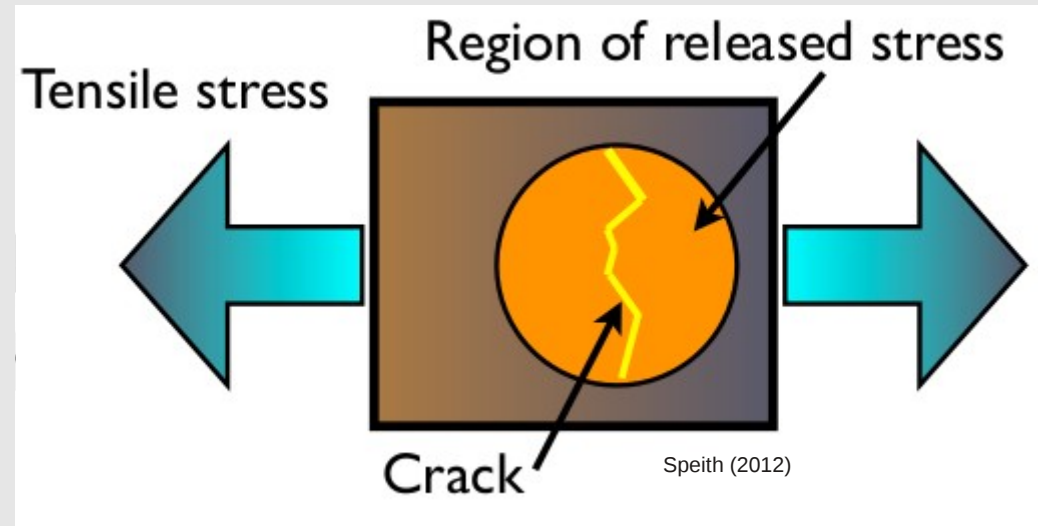
- ANEOS EOS

- Semi-analytical, not freely available

# Fracture model

- Large enough local **strain** causes **flaws** in the solids to develop into **cracks**
- Cracks grow at half the speed of sound until the local stress is relieved
- Grady & Kipp (1980) damage model:
  - damage  $D$  with  $0 \leq D \leq 1$
  - Stress  $\sim (1 - D)$
- Modified stress tensor:

$$\sigma_{\alpha\beta}^{\text{damaged}} = \begin{cases} -p\delta_{\alpha\beta} + (1 - D)S_{\alpha\beta} & , p \geq 0 \text{ (compression)} \\ -(1 - D)p\delta_{\alpha\beta} + (1 - D)S_{\alpha\beta} & , p < 0 \text{ (tension)} \end{cases}$$



# Flaw distribution

- The Grady-Kipp damage model assumes a probability distribution of flaws
- Weibull (1939) distribution:

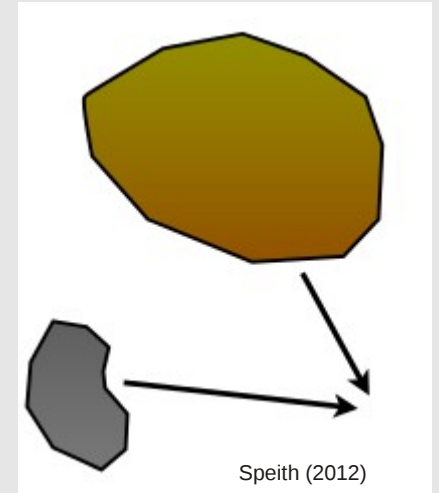
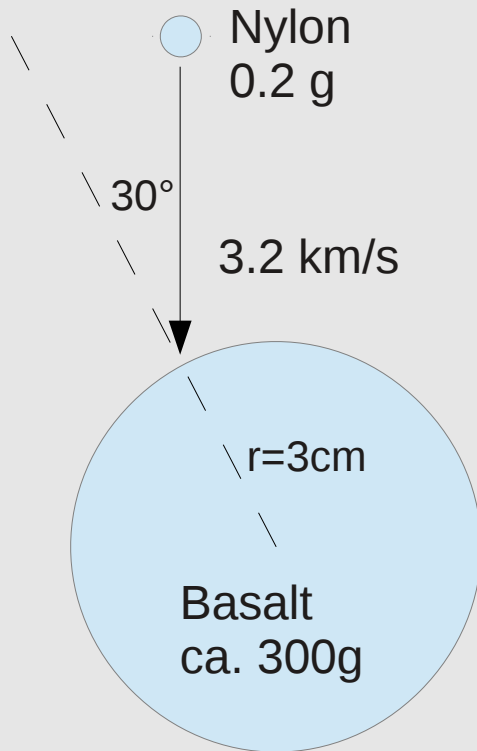
$$n(\varepsilon) = k \varepsilon^m$$

$n$  ... number of flaws per unit volume with activation thresholds  $< \varepsilon$

$k, m$  ... material parameters

- Distribution parameters not easily measurable...

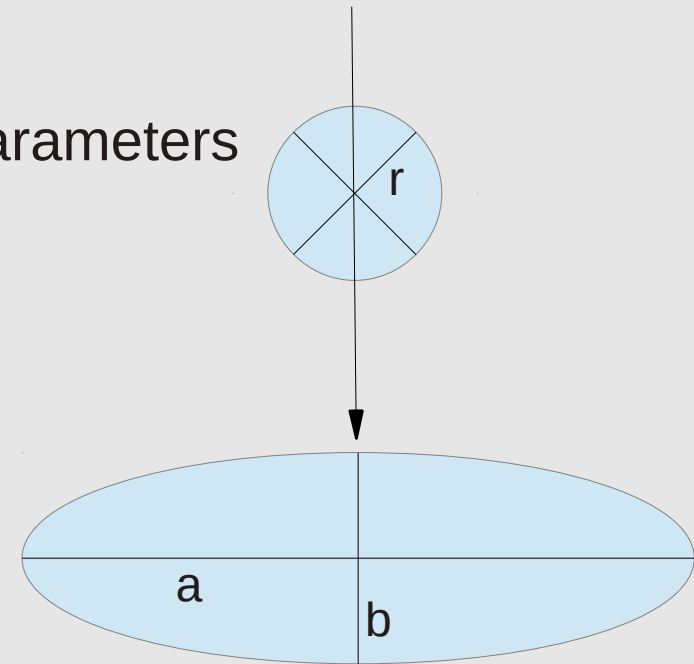
# Numerical tests





# First results

- Collisions of brittle bodies (basalt)
- Tillotson EOS, measured Weibull distribution parameters
- Projectile:
  - Spherical, e.g. small asteroid, 50cm radius
  - No flaws
- Target:
  - Spheroidal, e.g., irregular shaped small asteroid
    - Semi axes: 5m, 10m
- Impact velocity 1 km/s



**Table 2** (I) Material constants, cf. Benz & Asphaug (1999), (II) Weibull distribution parameters, cf. Nakamura et al. (2007) and Lange et al. (1984), respectively

	(I) $\mu$ (GPa)	$Y$ (GPa)	(II) $m$	$k$ ( $\text{m}^{-3}$ )
Basalt	22.7	3.5	16	$10^{61}$
Ice	2.8	1	9.1	$10^{46}$

Tillotson EOS parameters and vaporization energy levels adopted from Benz & Asphaug (1999)

	$\rho_0$ ( $\text{kg}/\text{m}^3$ )	$A$ (GPa)	$B$ (GPa)	$E_0$ (MJ/kg)	$E_{lv}$ (MJ/kg)	$E_{cv}$ (MJ/kg)	$a$	$b$	$\alpha$	$\beta$
Basalt	2700	26.7	26.7	487	4.72	18.2	0.5	1.50	5.0	5.0
Ice	917	9.47	9.47	10	0.773	3.04	0.3	0.1	10.0	5.0

Maindl et al. (2013)



# Challenge: material constants

- Material constants

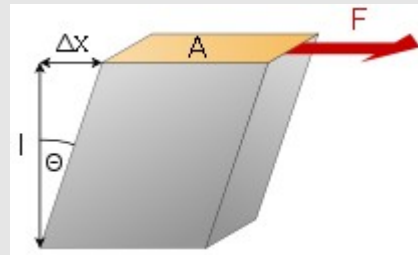
- Shear modulus  $\mu$

- 

- bulk modulus  $K$ , yield stress  $Y$

- Weibull distribution parameters

- EOS coefficients



**Table 2** (I) Material constants, cf. Benz & Asphaug (1999), (II) Weibull distribution parameters, cf. Nakamura et al. (2007) and Lange et al. (1984), respectively

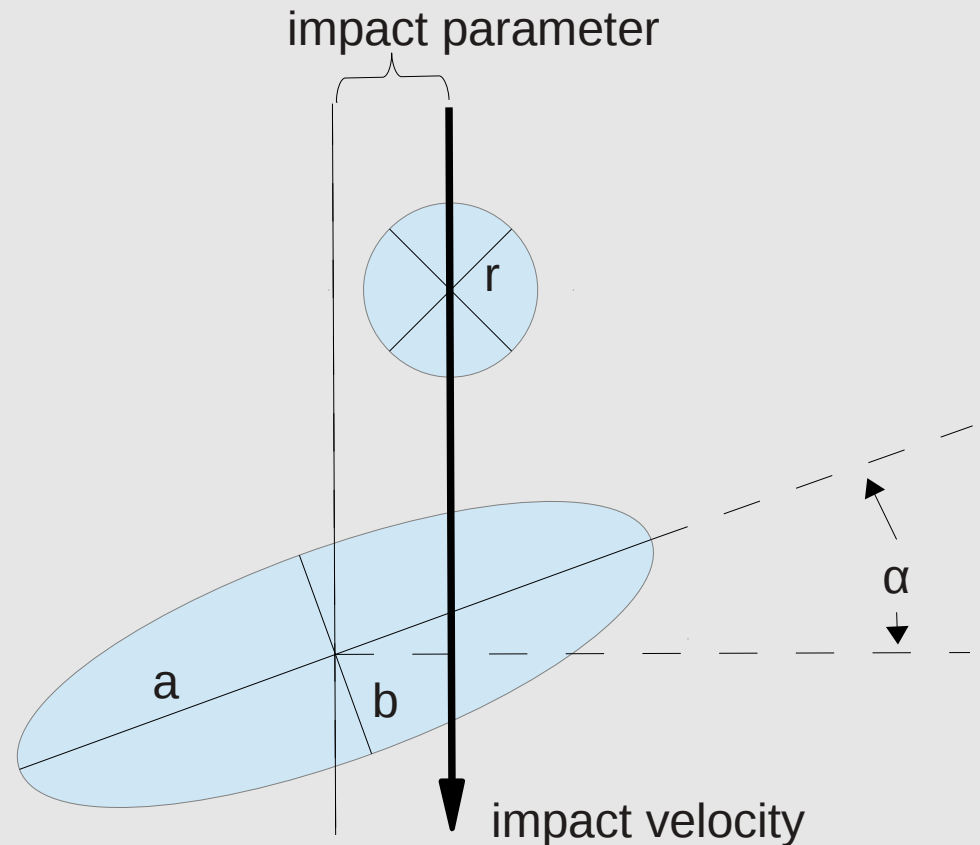
	(I)		(II)	
	$\mu$	$Y$	$m$	$k$
	(GPa)	(GPa)		( $\text{m}^{-3}$ )
Basalt	22.7	3.5	16	$10^{61}$
Ice	2.8	1	9.1	$10^{46}$

Tillotson EOS parameters and vaporization energy levels adopted from Benz & Asphaug (1999)

	$\rho_0$	$A$	$B$	$E_0$	$E_{iv}$	$E_{cv}$	$a$	$b$	$\alpha$	$\beta$
	( $\text{kg}/\text{m}^3$ )	(GPa)	(GPa)	(MJ/kg)	(MJ/kg)	(MJ/kg)				
Basalt	2700	26.7	26.7	487	4.72	18.2	0.5	1.50	5.0	5.0
Ice	917	9.47	9.47	10	0.773	3.04	0.3	0.1	10.0	5.0

# Outlook

- Measure fragmentation and merging
- Goal: water in early planetary systems
  - What influence does water content have?
    - Fragmentation
    - Merging
  - Water in/on protoplanets
  - Influence of different water/ice distributions
  - Porous bodies
  - Self gravitation?
  - Link to n-body



# References

Benz, W., Asphaug, E.: 1994, *Icar* 107, 98.

Benz, W., Asphaug, E.: 1999, *Icar* 142, 5.

Grady, D. E., Kipp, M. E.: 1980. Continuum modelling of explosive fracture in oil shale. *Int. J. Rock Mech. Min. Sci. Geomech. Abstr.* 17, 147.

Lange, M.A., Ahrens, T.J., Boslough, M.B.: 1984, *Icar* 58, 383.

Maindl, T.I., Schäfer, C., Speith, R., Süli, Á., Forgacs-Dajka, E., Dvorak, R.: 2013, SPH-based simulation of icy asteroid collisions. *Astron. Nachrichten*, in preparation.

Melosh, H.J.: 1989, *Impact Cratering – A Geologic Process*, Oxford Univ. Press, New York.

Monaghan, J.J.: 2000, SPH without a tensile instability. *Journal of Computational Physics* 159, 290.

Nakamura, A.M., Michel, P., Setoh, M.: 2007, *JGR* 112, E02001, doi:10.1029/2006JE002757.

NUI Galway: 2012, National University of Ireland, Galway, <http://www.nuigalway.ie/mechbio/research/meshfree.html>, accessed Sep 1, 2012.

Schäfer, C.: 2005, *Application of Smooth Particle Hydrodynamics to selected Aspects of Planet Formation*, Dissertation, Eberhard-Karls-Universität Tübingen.

Speith, R.: 2012, *Smoothed Particle Hydrodynamics*, Workshop at University of Vienna, Aug 1-3, 2012, unpublished.

Tillotson, J. H.: 1962. *Metallic equations of state for hypervelocity impact*. General Atomic Report GA-3216.

Weibull, W. A.: 1939. *A statistical theory of the strength of materials* [translated]. *Ingvetensk. Akad. Handl.* 151, 5.

# Thank you!